National Aeronautics and
Space Administration

NASA

HIGH-END COMPUTING CAPABILITY PORTFOLIO

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Tools Team Creates Report Automation Tool for Users

- The HECC Tools team developed a web-based Report Automation Tool that allows users to create their own ad hoc reports and queries located at reports.nas.nasa.gov.

- The new tool is more user friendly, easier to use, has more capabilities, and is much faster to execute compared to MicroStrategy, the previous tool used for HECC analytics reports.

- The tool was developed in Python/Django, with Oracle Database as the back end, and uses V2 Materialized View, which is already a normalized set of data.

- The Tools team completed the following key activities in order to develop the tool:
  - Gathered the requirements and investigated different usability/development options.
  - Created role-based credentials for login.
  - Built a coding framework.
  - Developed the complete functionality, such as create/edit/delete and run queries.
  - Built the SQL method that constructs the SQL query to run the report.
  - Included a capability where users can download the output to Excel or CSV files.

- The Reports Automation Tool was made available to users on August 27, and the feedback from users has been very positive.

IMPACT: The development and successful implementation of a Reports Automation Tool provides improved features and performance for HECC users to create their own reports.

Screenshot showing the Query Output page for the Report Automation Tool created for HECC users.

New DDN Filesystem Now in Production

- New Data Direct Networks (DDN) filesystems are now in production and available to users. The new storage capability provides about 50% more capacity and a 100% increase in write speeds.

- Historically, HECC compute resources have expanded faster than storage; these new storage systems will help alleviate that imbalance.
  - DataDirect Networks (DDN): 3,600 18-terabyte (TB), 7.2K-RPM drives, 12-gigabytes/second Serial Attached SCSI (SAS), 4K-hard disk drive (HDD) module, 240 15.36 TB-1 Drive Writes Per Day (DWPD) dual-port NVMe self-encrypting drive (SED)-capable, 4K-solid-state drive (SSD) module.
    - Two large filesystems, each with: Total usable HDD of 18 petabytes (PB); total usable Non-Volatile Memory Express (NVMe) of 1 PB.
    - One smaller filesystem: Total usable HDD of 9 PB; total usable NVMe of 500 TB.

- User data migration to the new Data Direct Networks (DDN) filesystems from HECC's older file systems is in progress and users are already reporting a significant performance increase.

- These new filesystems are coming online at an opportune time, with the New Operational Period (NOP) for FY 2022 starting on October 1, 2021.

IMPACT: The new HECC filesystems will provide users with more storage space and much faster performance compared to the older filesystems.


Photo of the newly installed DataDirect Networks (DDN) storage hardware at the NASA Advanced Supercomputing facility. *Jonathan LaBounty, ASRC*

HECC Support Teams Hold Final 2021 Virtual User Meeting

- HECC completed the final of three virtual user meetings aimed at highlighting and promoting the project's extensive resources and services.

- The meeting was attended by 46 users, 3 representatives from HQ/HEC/SMD, and 18 staff members.

- The User Services team is now drafting a report that will cover user feedback and summarize what was learned.

- Several adjustments were made to improve the meeting structure and participant engagement, based on experiences from the previous meetings, including: holding Q&A at the end of the meeting vs. office hours; better utilization of the chat; and staff staying on during the break for casual discussion (working lunch).

- The virtual meetings allowed HECC to reach a larger number of users, many of whom would not have been able to attend otherwise. However, it is agreed they are not an adequate replacement for in-person gathering of feedback and requirements. HECC will adopt a hybrid approach to outreach, when possible, with in-person meetings and a virtual session open to all users.

IMPACT: User outreach is critical to ensuring that scientists and engineers can make the most of their compute resources and have the opportunity to give HECC staff a better understanding of users' needs.
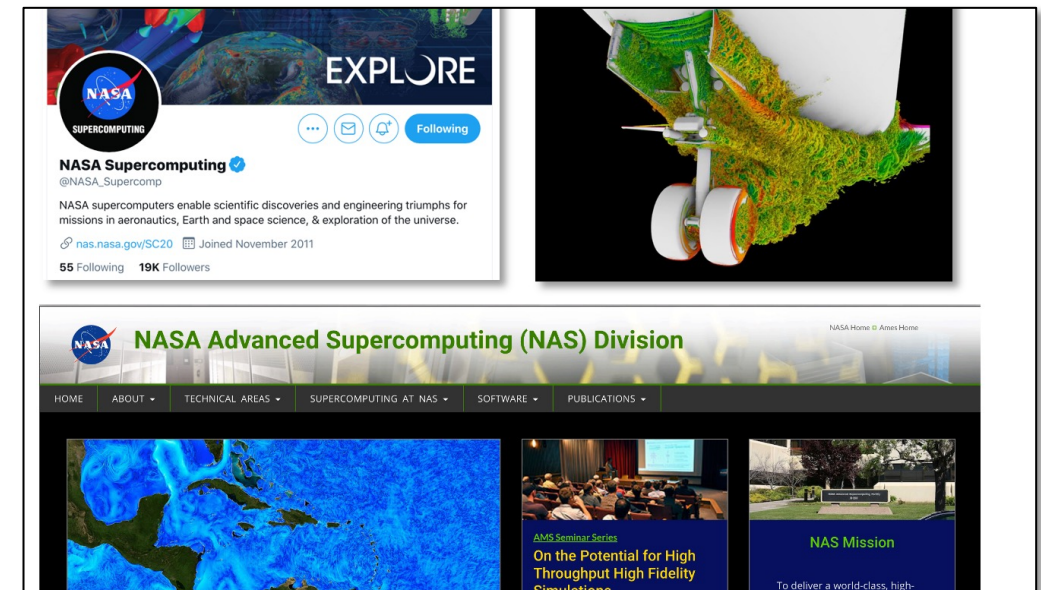

Slide from the HECC Publications and Media presentation giving examples of how the group can promote and amplify user's work. All slides will be made available on the HECC website. *Katie Pitta, NASA/Ames*

Molecular Dynamics of the SARS-CoV-2 Spike Protein*

- As part of the COVID-19 High-Performance Computing (HPC) Consortium, scientists at the University of Minnesota and Virginia Commonwealth University used Pleiades to investigate the energetics and dynamics that occur within the SARS-CoV-2 virus's spike protein, which plays a key role in binding to human epithelial cells and enabling the virus to infect the body.
  - The spike protein contains three identical subunits, known as protomers, that each contain a molecular "latch" that plays an important role in binding to epithelial cells during the cellular infection process.
  - The researchers identified the amino acids that appear to be involved in this "latch," along with insights into the molecular dynamics involved in the stability of the protein, which could lead to the development of treatments—such as peptide-based inhibitors that could destabilize the protein or help prevent binding to host cell proteins.

- Simulating the molecular dynamics of the spike protein—which is composed of over 51,000 atoms—is extremely computationally intensive, requiring the use of high-performance computing resources. Future work includes running simulations of systematic mutations to the molecular latch in order to characterize its role in protomer stability in greater detail.

* HECC provided supercomputing resources and services in support of this work

IMPACT: NASA provided access to HECC resources and expertise as part of the HPC Consortium to support researchers in the fight to understand the pandemic and to develop treatments and vaccines.
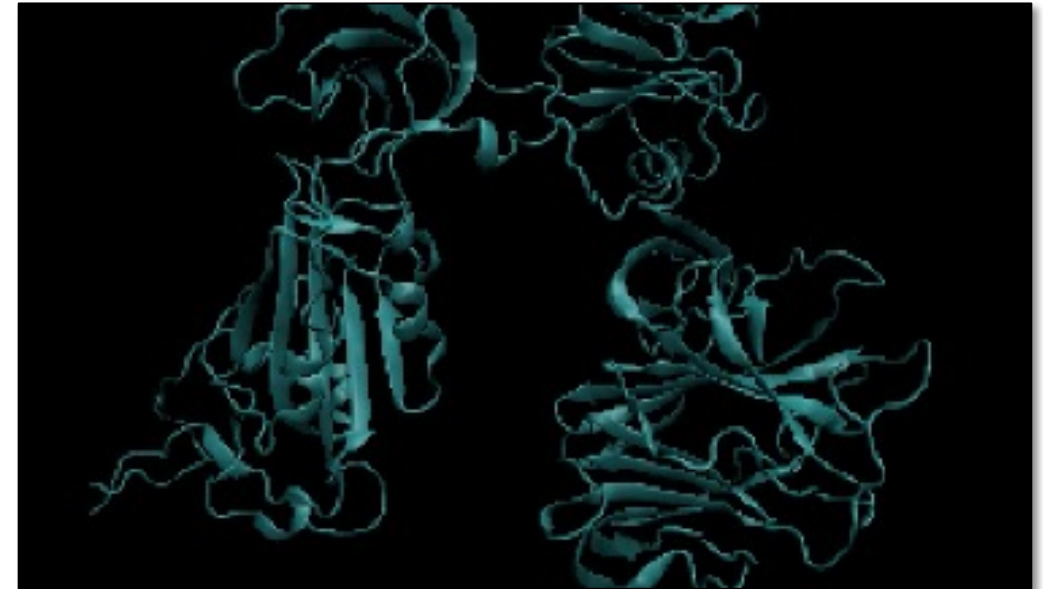
Visualization showing protein fluctuations of two alloforms of SARS-CoV-2 spike protein protomers. The mutant protomer is deliberately targeting a component of the molecular "latch," which demonstrates the latch's role in maintaining an up or down state of the spike protein's protomer. *Oscar Bastidas, University of Minnesota; Michael Peters, Virginia Commonwealth University*

Generating Aerodynamic Databases for the X-57 Maxwell*

- A collaboration between NASA's Ames Research Center, Armstrong Flight Research Center, and Langley Research Center has demonstrated the ability of computational fluid dynamics (CFD) solvers to accurately predict the complex aerodynamic characteristics of NASA's X-57 Maxwell, using HECC supercomputing resources. The electric aircraft concept is designed to achieve a 5x reduction in energy consumption when compared to traditional fossil-fuel-powered turboprop propulsion.

- In order to construct aerodynamic databases for the X-57, thousands of CFD simulations have been conducted for multiple aircraft configurations, flight conditions, and propulsion settings. Multiple time-dependent computations were also performed to assess the dynamic stability of the aircraft under forced roll, pitch, and yaw oscillations.

- Simulations using the in-house developed Launch Ascent and Vehicle Aerodynamics (LAVA) flow solver were performed by solving steady and unsteady Reynolds-Averaged Navier-Stokes (RANS) equations with a structured curvilinear mesh paradigm, with more than 2,500 flight conditions simulated to date. Initial simulations served as a successful validation of CFD predictions, and solutions from multiple solvers were compared to verify that predictions were consistent. In addition to helping engineers design and validate configurations, the X-57 databases will also be used to develop a flight simulator model used to train pilots for safe flight.

* HECC provided supercomputing resources and services in support of this work.

IMPACT: Key lessons learned during the generation of the X-57 databases will be valuable for future mission-critical NASA projects, including procedures for verification and validation to ensure subsequent database simulations are optimal in terms of accuracy and computational efficiency.
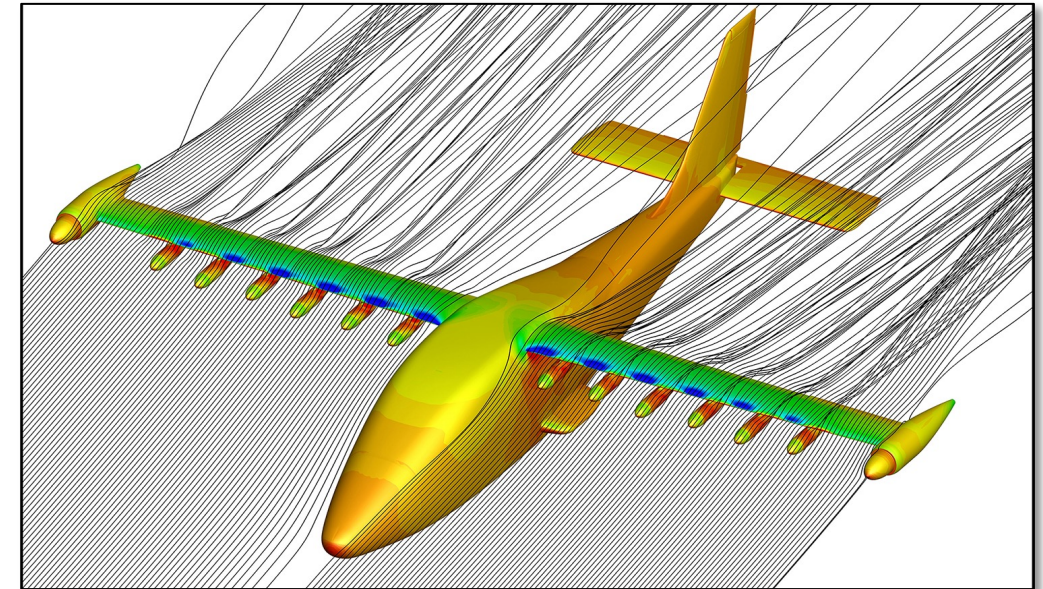
An X-57 flow visualization is shown for a sample CFD solution using the LAVA curvilinear flow solver. Surface pressure distribution is shown (blue and red contours correspond to high and low pressure, respectively) with streamlines showing the effects of the high-lift propellers. *Jared Duensing, Cetin Kiris, NASA/Ames*

Papers

- "**HD 183579b: A Warm Sub-Neptune Transiting a Solar Twin Detected by TESS**," T. Gan, et al., Monthly Notices of the Royal Astronomical Society, vol. 507, issue 2, published August 2, 2021. *
  https://academic.oup.com/mnras/article-abstract/507/2/2220/6335490

- "**Scaling Theory of Three-Dimensional Magnetic Reconnection Spreading**," M. Arencibia, et al., Physics of Plasmas, vol. 28, issue 8, published August 2, 2021. *
  https://aip.scitation.org/doi/abs/10.1063/5.0052189

- "**TESS Giants Transiting Giants I: A Non-Inflated Hot Jupiter Orbiting a Massive Subgiant**," N. Saunders, et al., arXiv:2108.02294 [astro-ph.EP], August 4, 2021. *
  https://arxiv.org/abs/2108.02294

- "**Spatiotemporal Methane Emission from Global Reservoirs**," M. Johnson, et al., Journal of Geophysical Research: Biogeosciences, vol. 126, issue 8, August 4, 2021. *
  https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2021JG006305

- "**Using Cosmological Simulations and Synthetic Absorption Spectra to Assess the Accuracy of Observationally Derived CGM Metallicites**," R. Marra, et al., arXiv:2021.03254 [astro-ph.GA], August 6, 2021. *
  https://arxiv.org/abs/2108.03254

* HECC provided supercomputing resources and services in support of this work

Papers (cont.)

- "**Development of Adjoint-Based Ocean State Estimation for the Amundsen and Bellingshausen Seas and Ice Shelf Cavities using MITgcm-ECCO (66j)**," Y. Nakayama, et al., Geosciences Model Development, vol. 14, issue 8, published online August 6, 2021. *
https://gmd.copernicus.org/articles/14/4909/2021/gmd-14-4909-2021.html

- "**Fossil Fuel CO_2 Emissions Over Metropolitan Areas from Space: A Multi-Model Analysis of OCO-2 Data over Lahore, Pakistan**," R. Lei, Remote Sensing of Environment, vol. 264, published online August 10, 2021. *
https://www.sciencedirect.com/science/article/pii/S003442572100345X

- "**The Plasma Environment Surrounding the Reiner Gamma Magnetic Anomaly**," J. Deca, et al., Journal of Geophysical Research: Space Physics, vol. 126, issue 9, August 11, 2021. *
https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2021JA029180

- "**A Pair of Warm Giant Planets Near the 2:1 Mean Motion Resonance around the K-dwarf Star TOI-2202**," T. Trifonov, et al., arXiv:2108.05323 [astro-ph.EP], August 11, 2021. *
https://arxiv.org/abs/2108.05323

- "**Data-Driven Expectations for Electromagnetic Counterpart Searches Based on LIGO/Virgo Public Alerts**," P. Petrov, et al., arXiv:2108.07277 [astro-ph.HE], August 16, 2021. *
https://arxiv.org/abs/2108.07277

* HECC provided supercomputing resources and services in support of this work

Papers (cont.)

- "**Large Eddy Simulation of Premixed Turbulent Combustion Using a Non-Adiabatic, Strain-Sensitive Flamelet Approach**," Y. Tang, V. Raman, Combustion and Flame, vol. 234, published online August 18, 2021. *
  https://www.sciencedirect.com/science/article/abs/pii/S0010218021003989

- "**Simulation Study of Hatch Spacing and Layer Thickness Effects on Microstructure in Laser Powder Bed Fusion Additive Manufacturing using Texture-Aware Solidification Potts Model**," J. Pauza, A. Rollett, Journal of Materials Engineering and Performance, August 19, 2021. *
  https://link.springer.com/article/10.1007/s11665-021-06110-7

- "**Physical Properties and Real Nature of Massive Clumps in the Galaxy**," Z.-J. Lu, et al., arXiv:2108.08981 [astro-ph.GA], August 20, 2021. *
  https://arxiv.org/abs/2108.08981

- "**Bursty Magnetic Reconnection at the Earth's Magnetopause Triggered by High-Speed Jets**," J. Ng, L.-J. Chen, Y. Omelchenko, arXiv:2108.09419 [physics.space-ph], August 21, 2021. *
  https://arxiv.org/abs/2108.09419

- "**Masses and Compositions of the Three Small Planets Orbiting the Nearby M-dwarf L231-32 (TOI-270) and the M-dwarf Radius Valley**," V. Van Eylen, et al., Monthly Notices of the Royal Astronomical Society, vol. 507, issue 2, published online August 24, 2021. *
  https://academic.oup.com/mnras/article/507/2/2154/6356971

* HECC provided supercomputing resources and services in support of this work

Papers (cont.)

- "**Photospheric Prompt Emission from Long Gamma Ray Burst Simulations—II. Spectropolarimetry**," T. Parsotan, D. Lazzati, arXiv:2108.11412 [astro-ph.HE], August 25, 2021. *
  https://arxiv.org/abs/2108.11412

- "**Two Steps Forward and One Step Sideways: The Propagation of Relativistic Jets in Realistic Binary Neutron Star Merger Ejecta**," D. Lazzati, et al., The Astrophysical Journal Letters, vol. 918, published August 25, 2021. *
  https://iopscience.iop.org/article/10.3847/2041-8213/ac1794/pdf

- "**Visible-light Phase Curves from the Second Year of the TESS Primary Mission**," I. Wong, et al., The Astronomical Journal, vol. 162, no. 4, August 31, 2021. *
  https://iopscience.iop.org/article/10.3847/1538-3881/ac0c7d

* HECC provided supercomputing resources and services in support of this work

News and Events

- **NAS Models Illuminate Understanding of Rotating Stars**, *NASA Advanced Supercomputing Division*, August 9, 2021— New research led by NASA provides a closer look at a nearby star thought to resemble our young Sun. Using the Pleiades supercomputer at the NAS facility, the researchers performed simulations of the star Kappa 1 Ceti with an updated model and data inputs from a variety of space missions.
https://www.nas.nasa.gov/pubs/stories/2021/feature_models_of_rotating_stars.html

News and Events: Social Media

- **Coverage of NAS Stories**
  - Heliophysics Model Feature Story
    - NAS: [Twitter](#) 8 retweets, 12 favorites.
  - SiliCon 2021 NASA Panel
    - NAS: [Twitter](#) 2 retweets, 6 favorites.

HECC Utilization
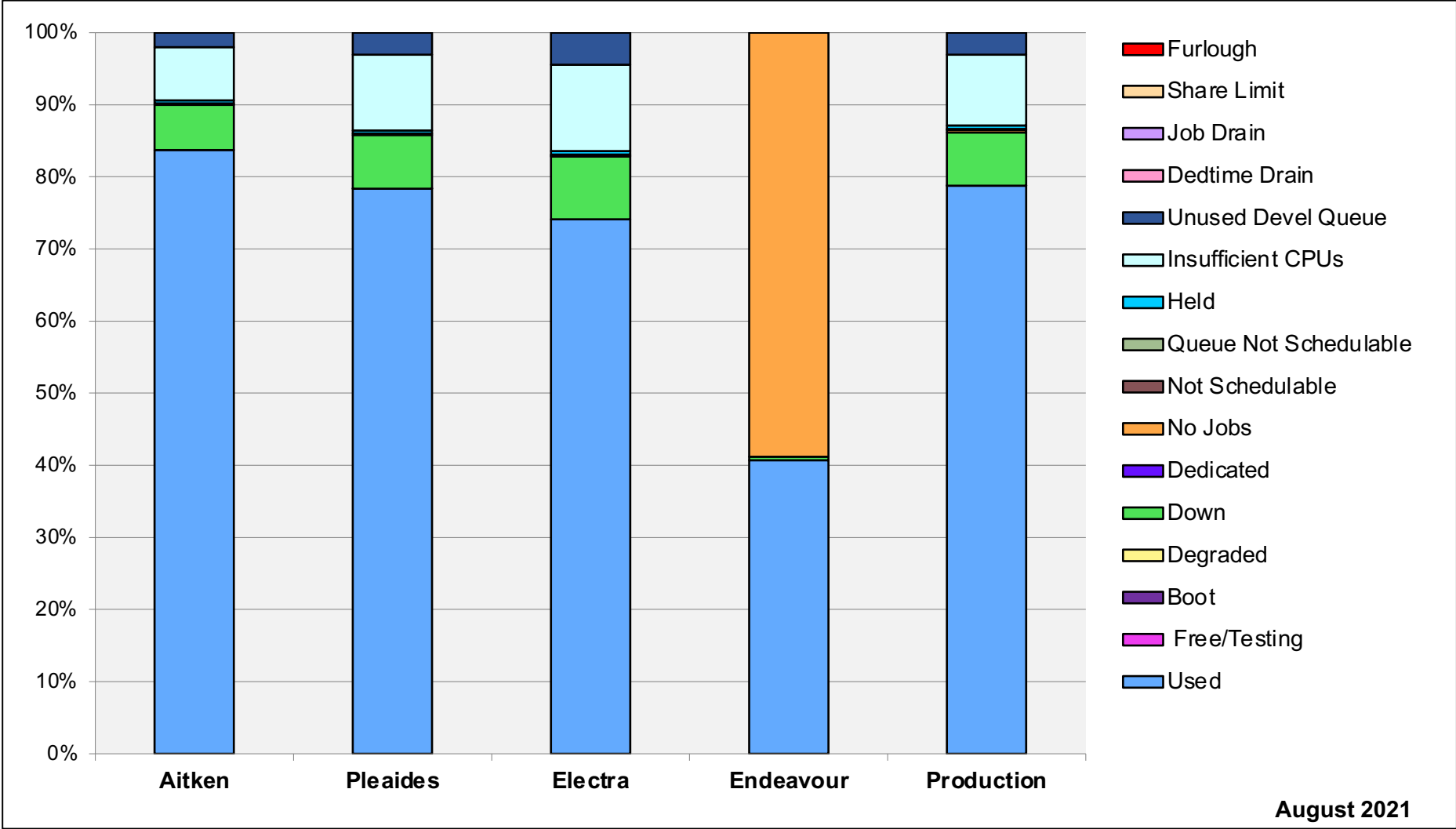
HECC Utilization Normalized to 30-Day Month

HECC Utilization Normalized to 30-Day Month

① 4 Cascade Lake E cells introduced into Aitken

② 8 Rome Apollo racks introduced into Aitken

③ Endeavour replaced with new hardware

④ Merope retired, Annual Maintenance
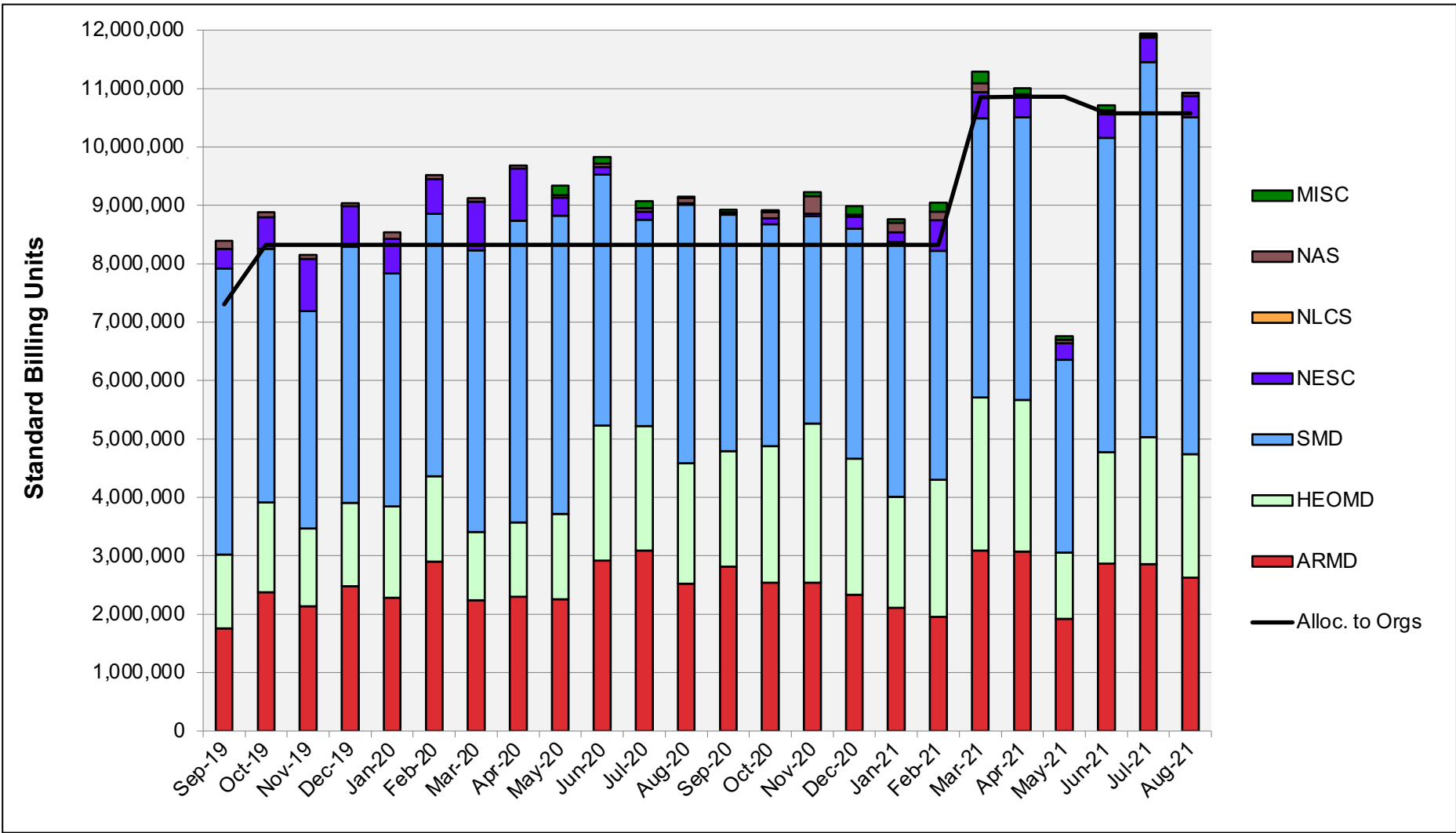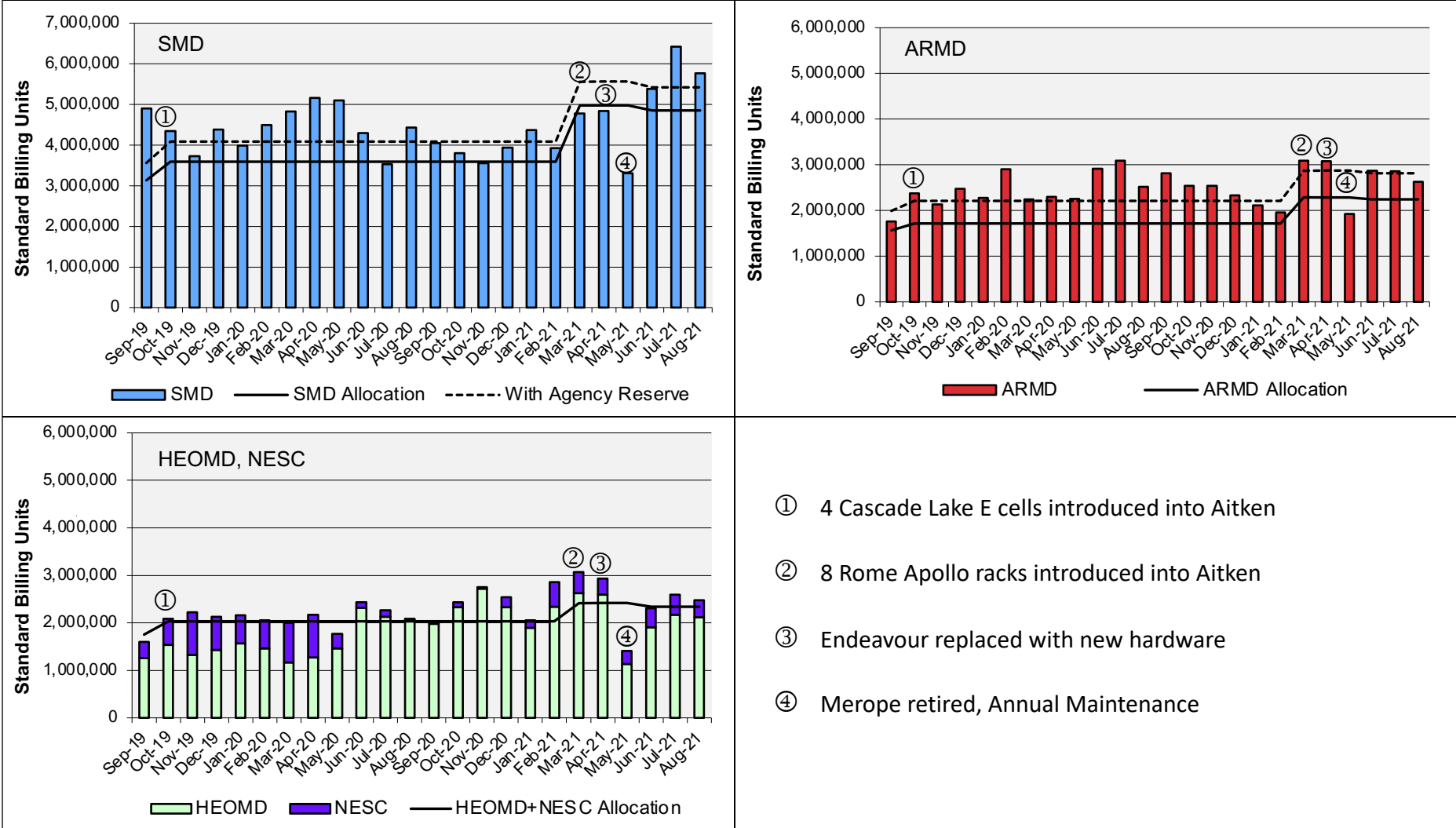
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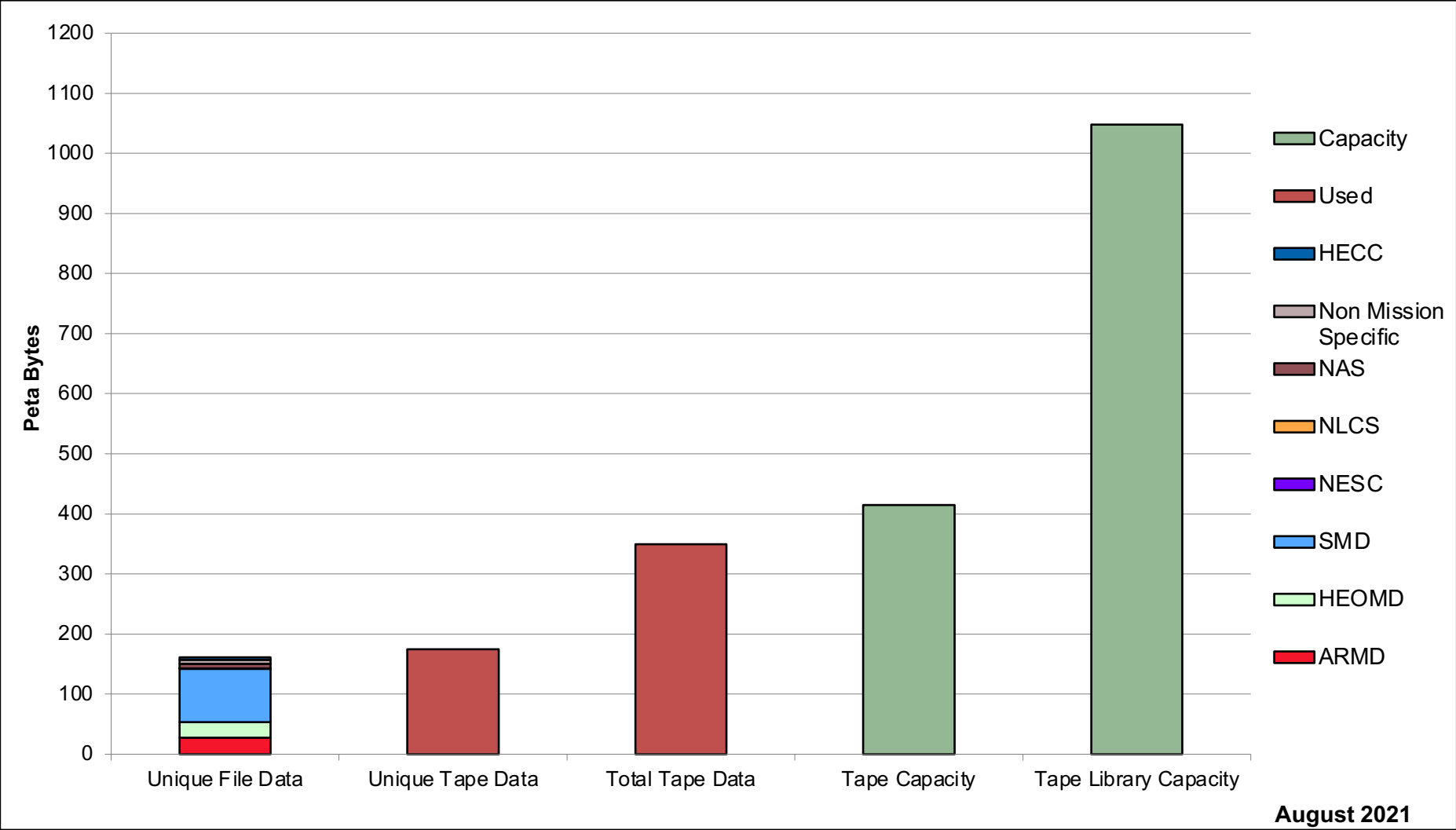
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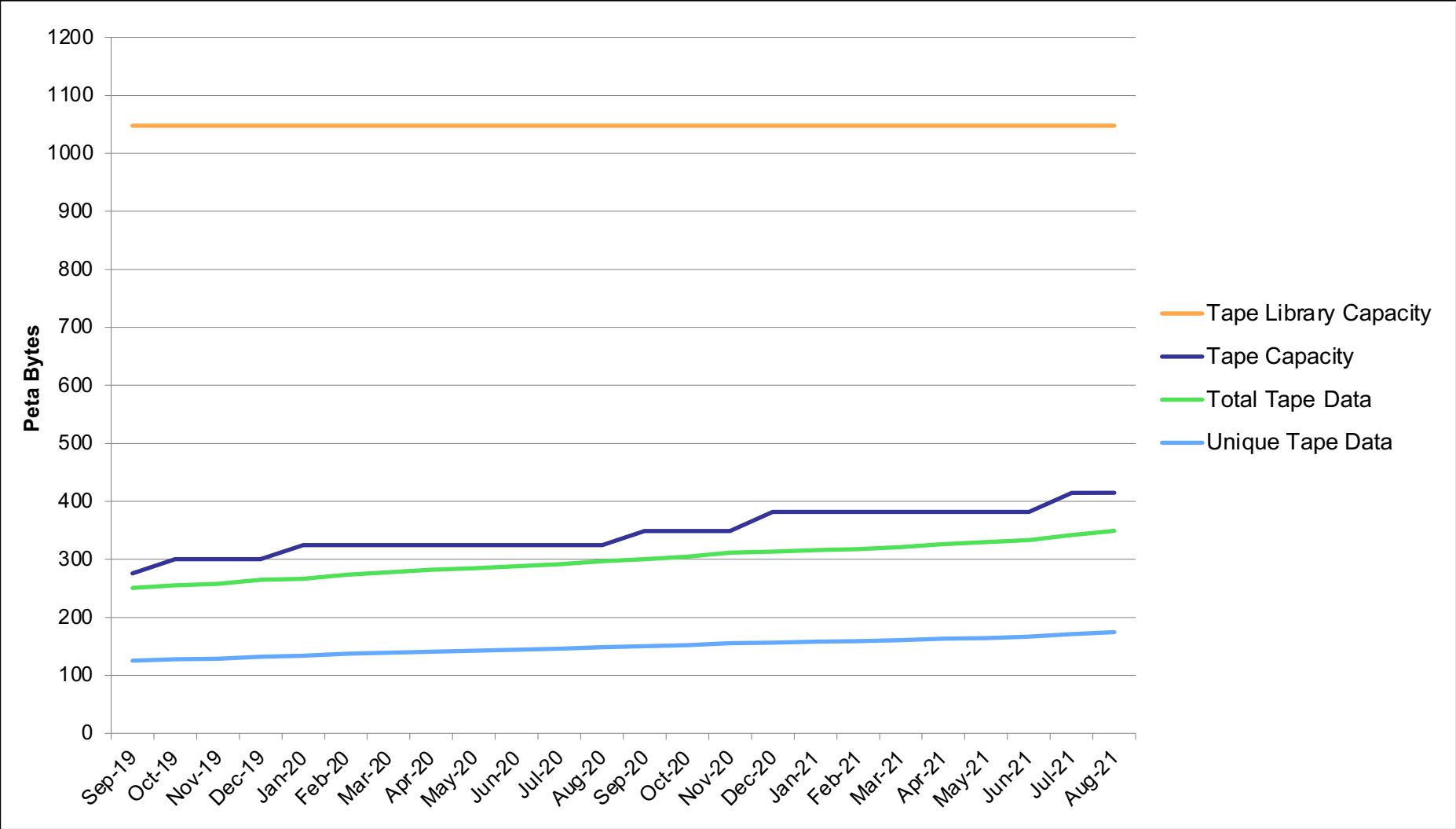
Pleiades: SBUs Reported, Normalized to 30-Day Month
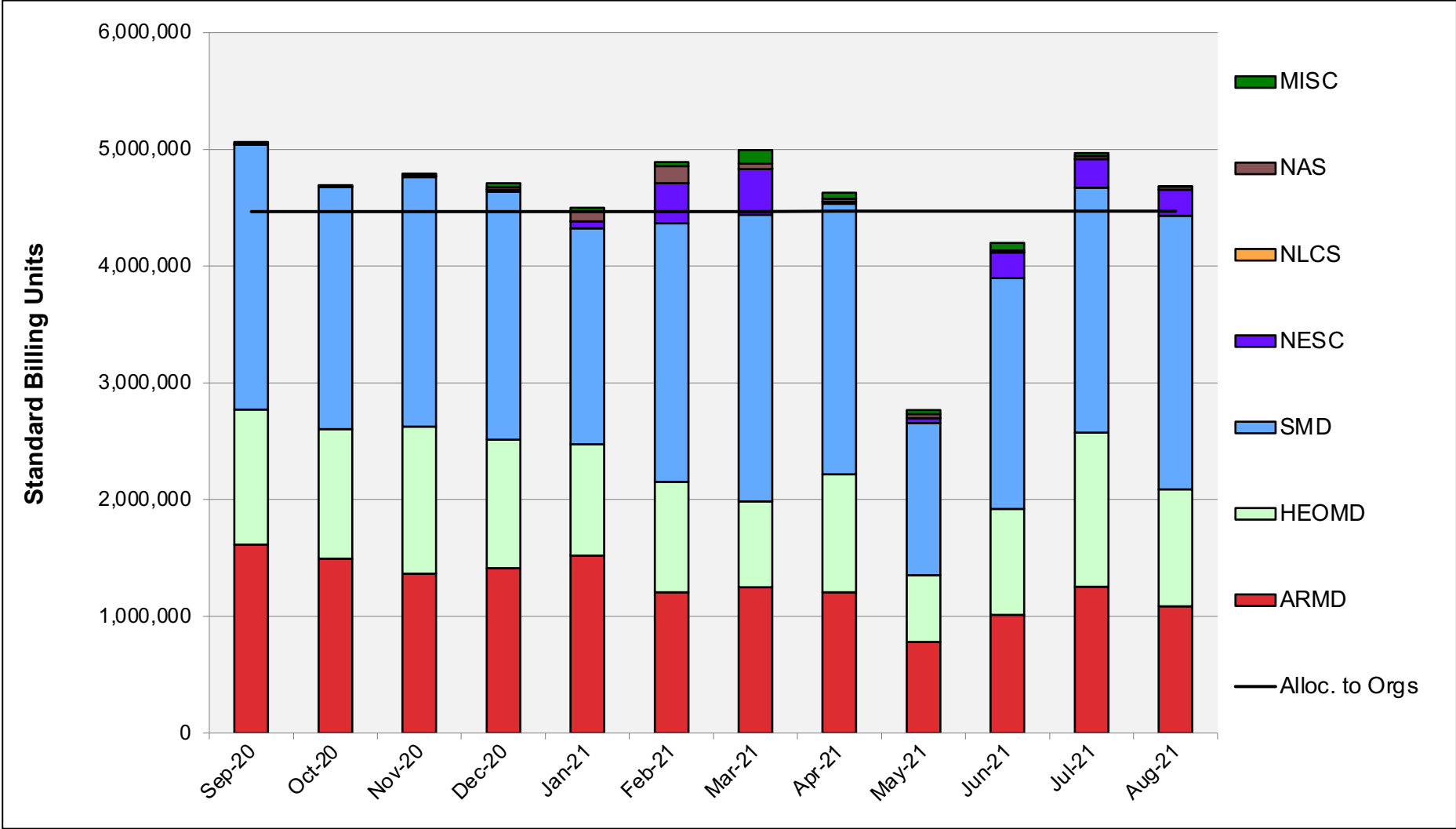
Pleiades: Devel Queue Utilization
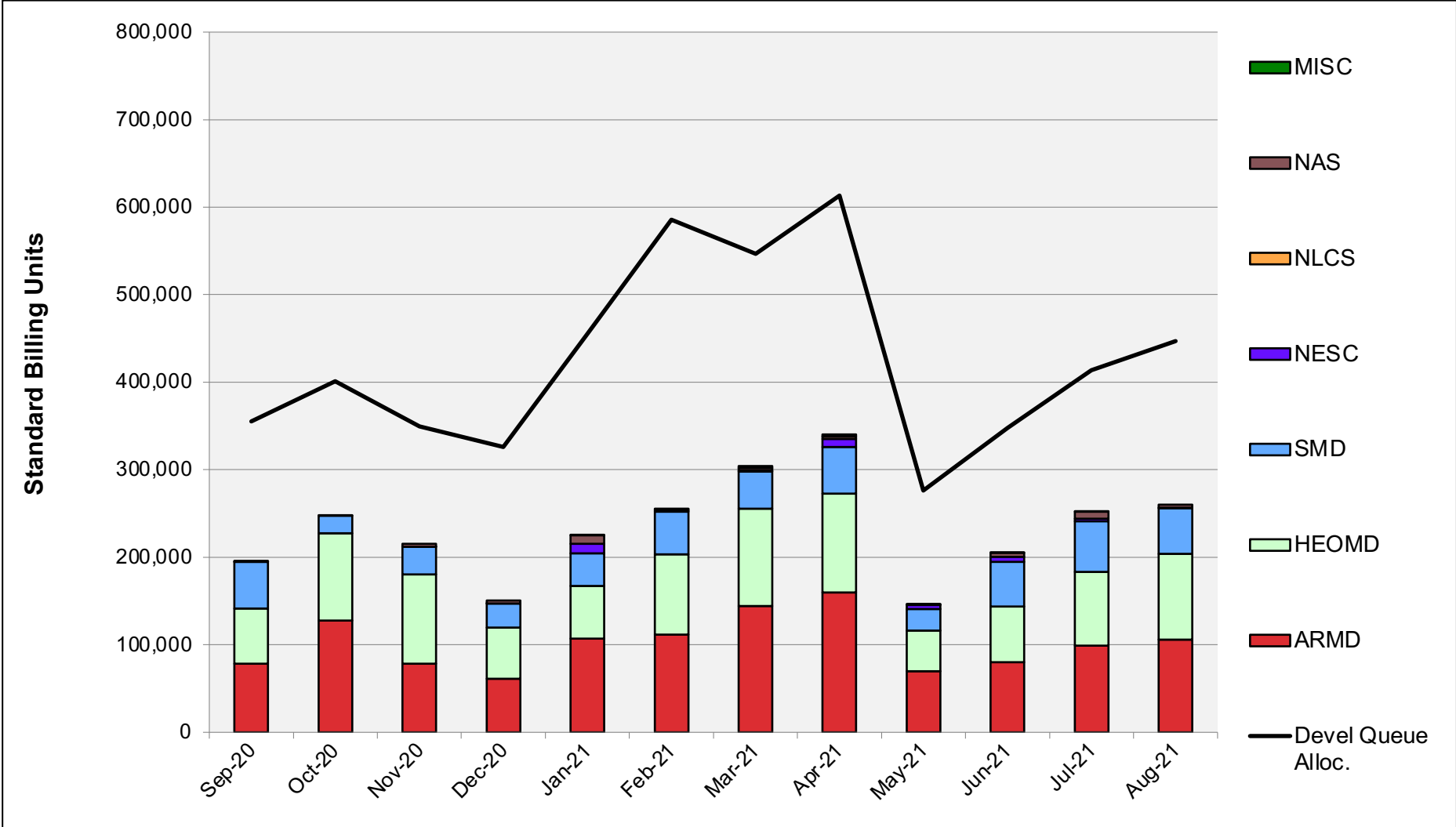
Pleiades: Monthly Utilization by Job Length
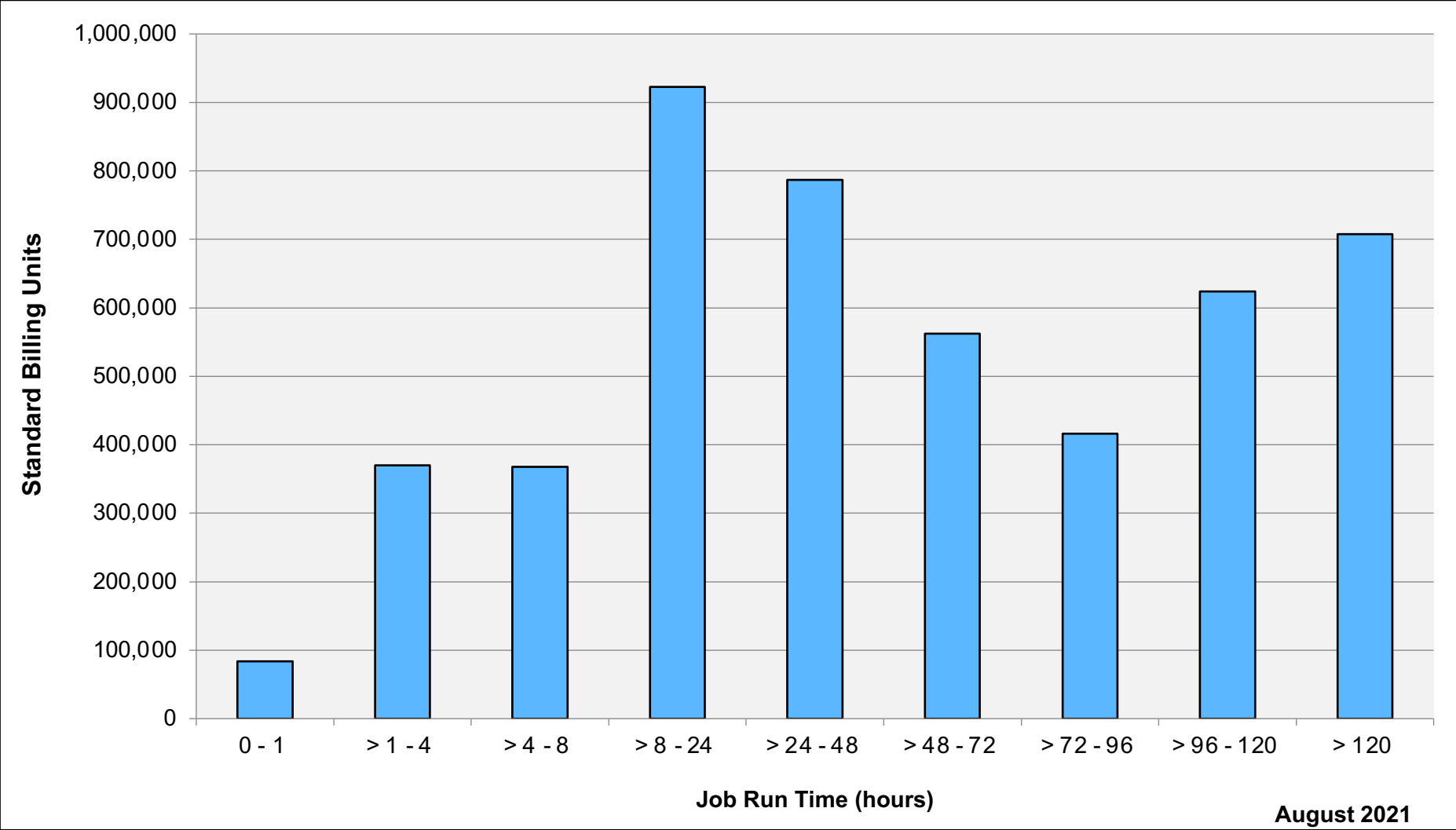
August 2021

Pleiades: Monthly Utilization by Job Size

August 2021

Pleiades: Monthly Utilization by Size and Length

August 2021
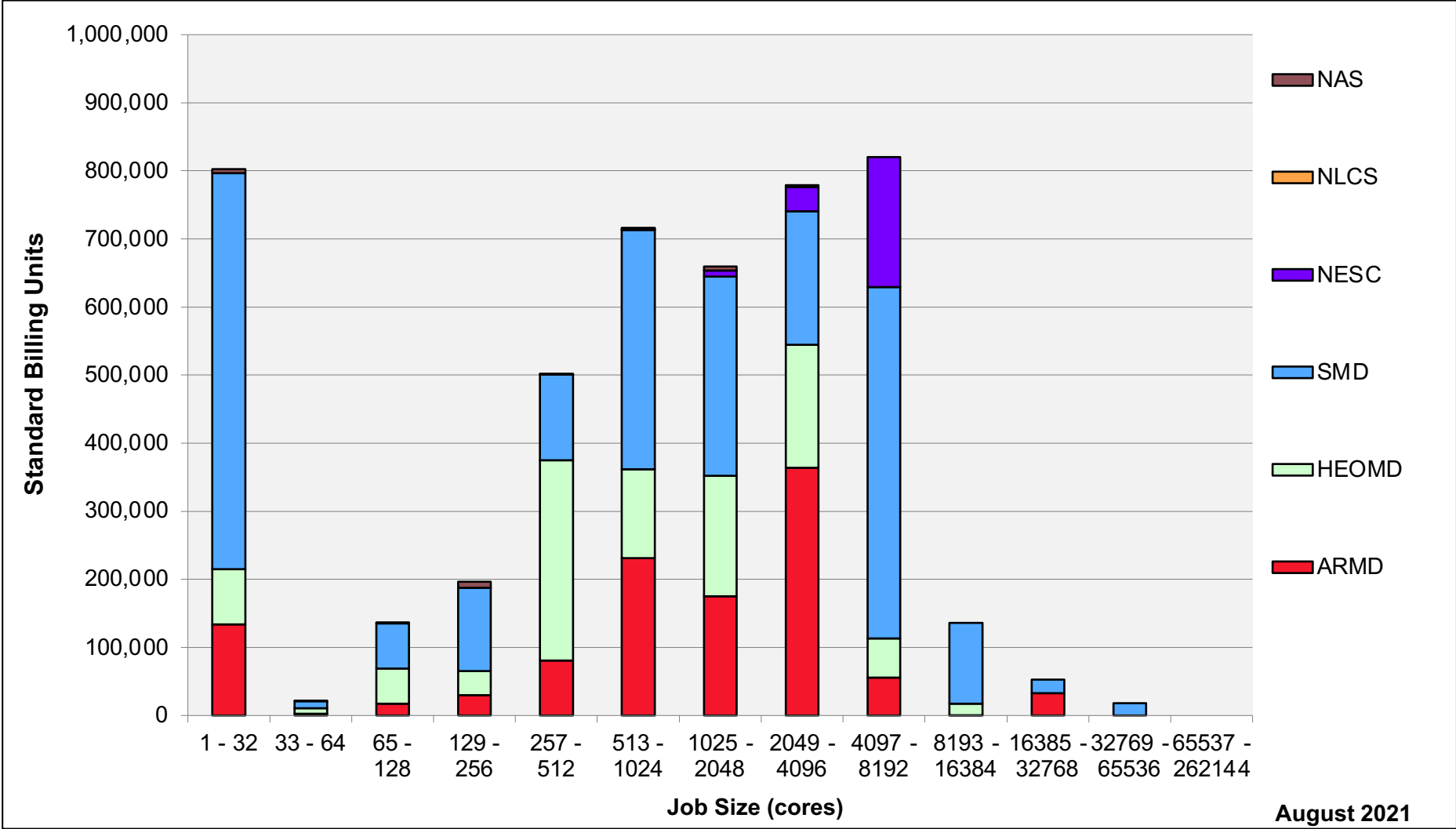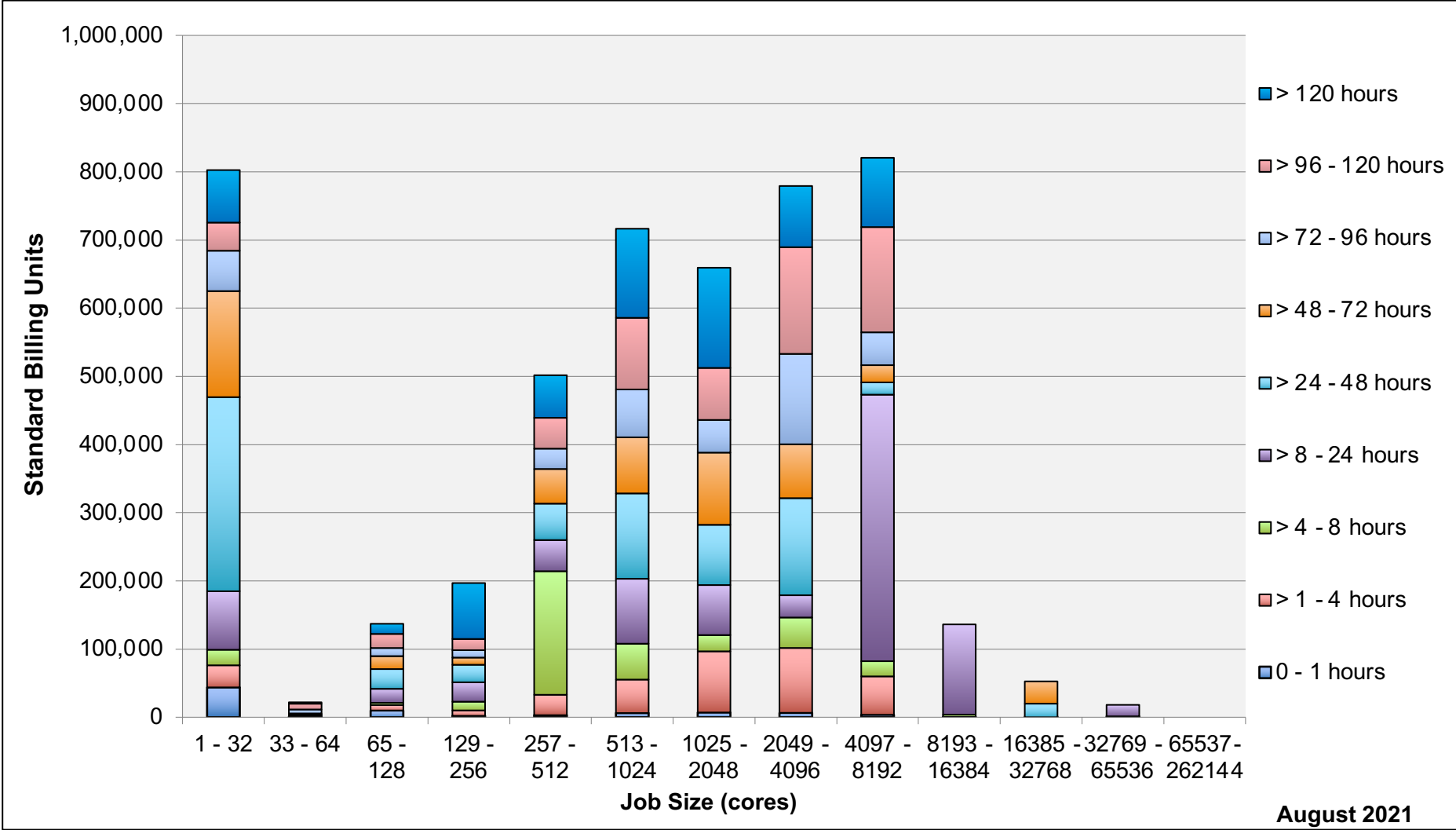
Pleiades: Average Time to Clear All Jobs
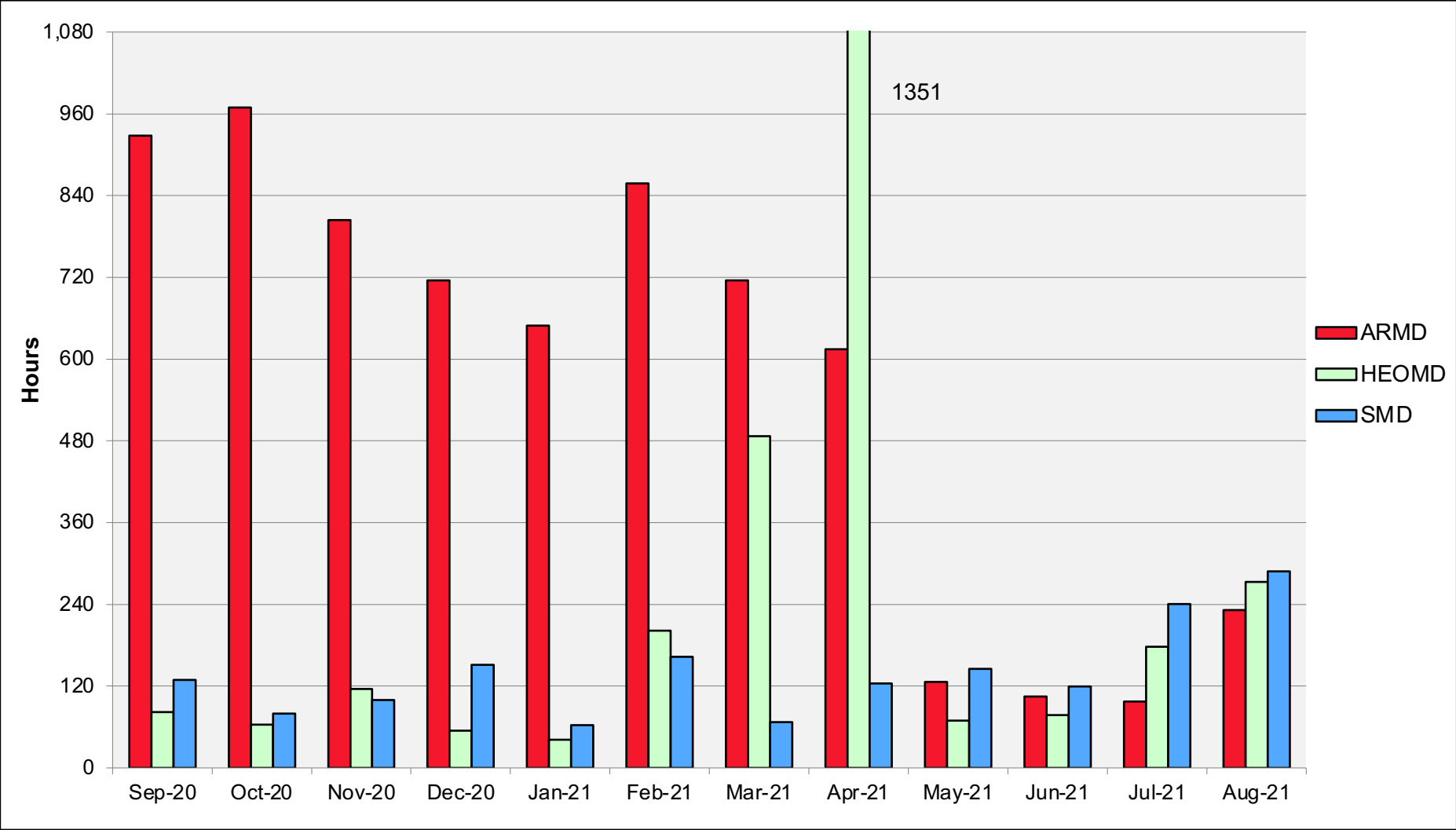
Pleiades: Average Expansion Factor
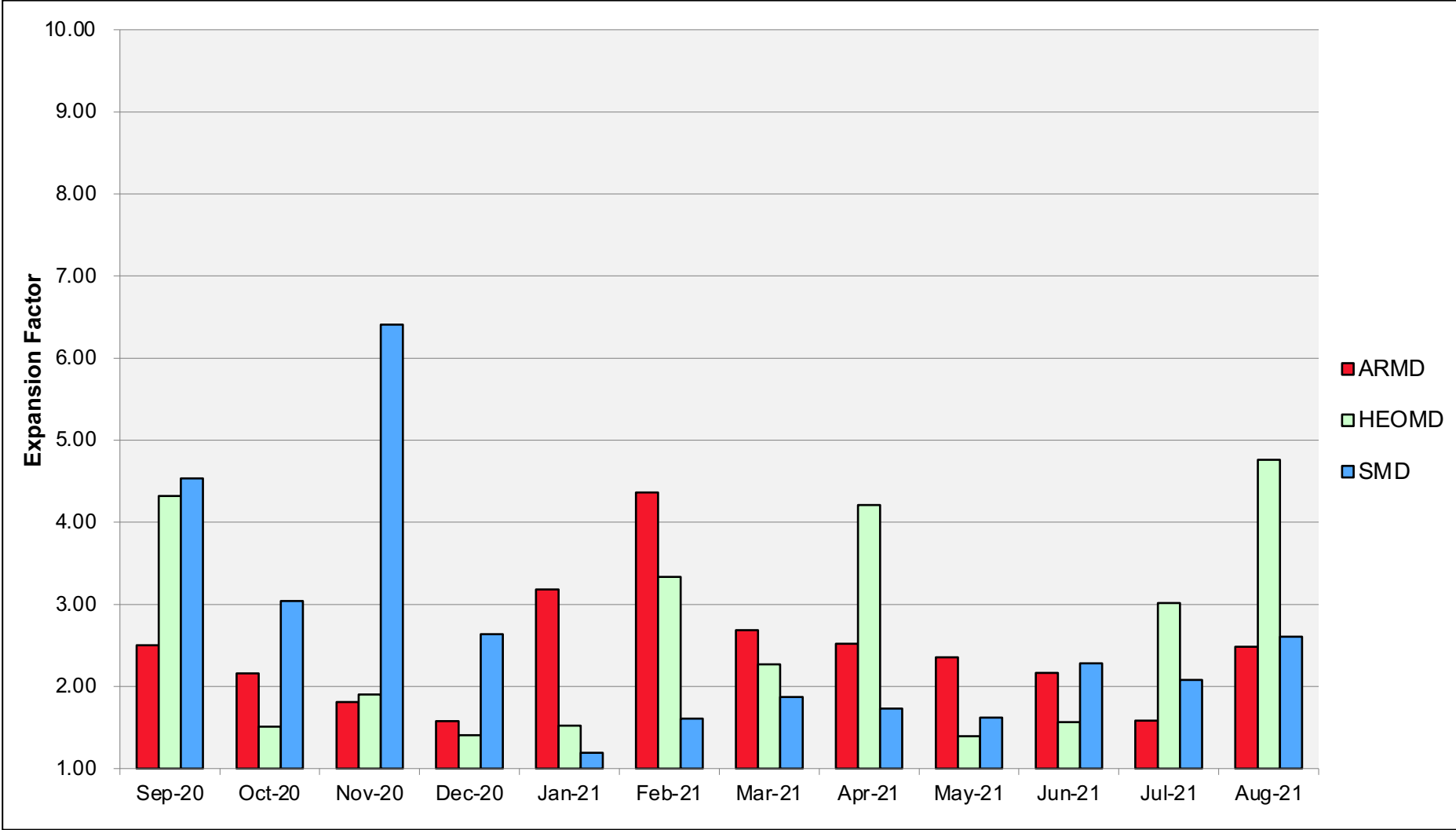
Aitken: SBUs Reported, Normalized to 30-Day Month
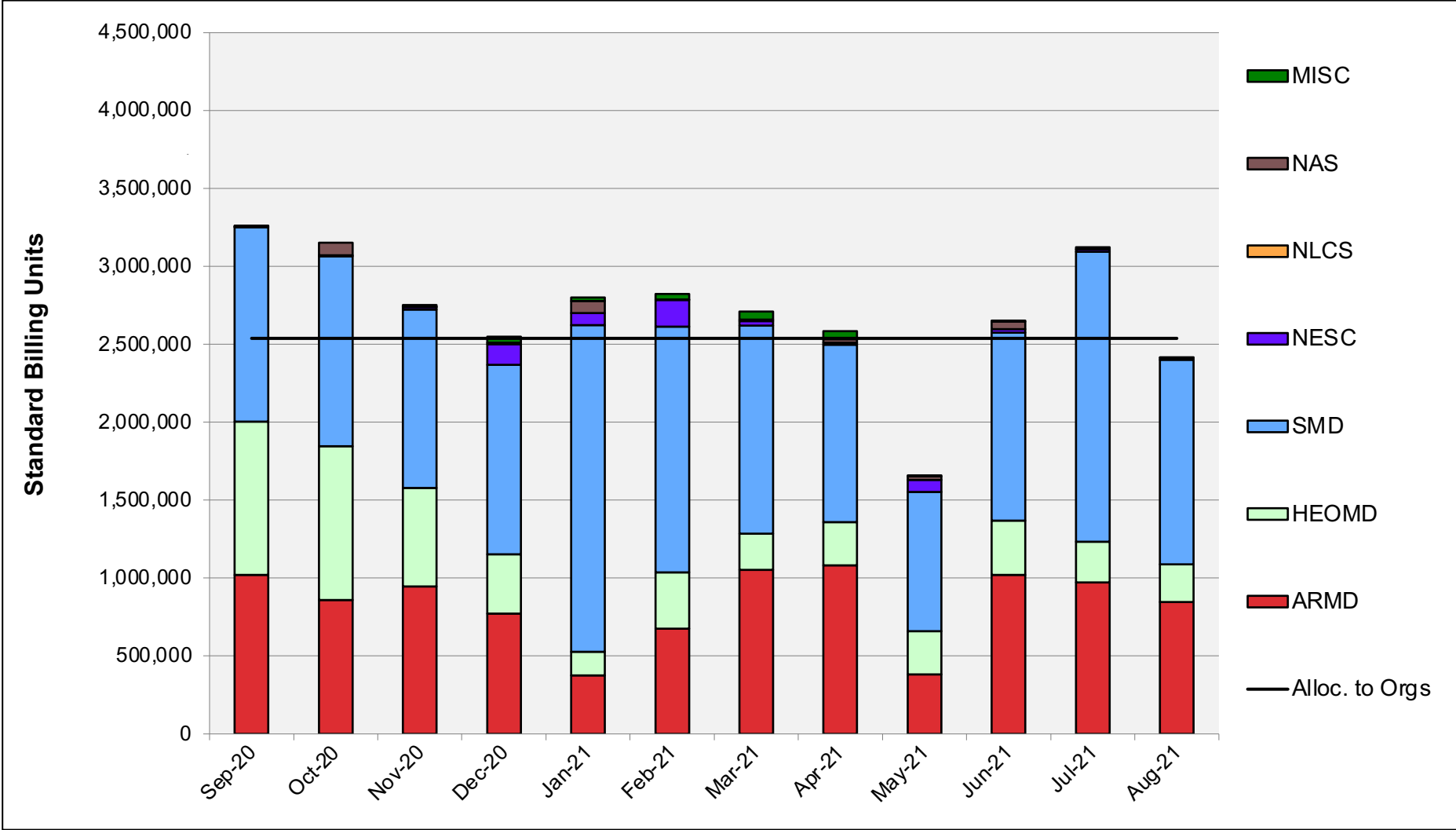
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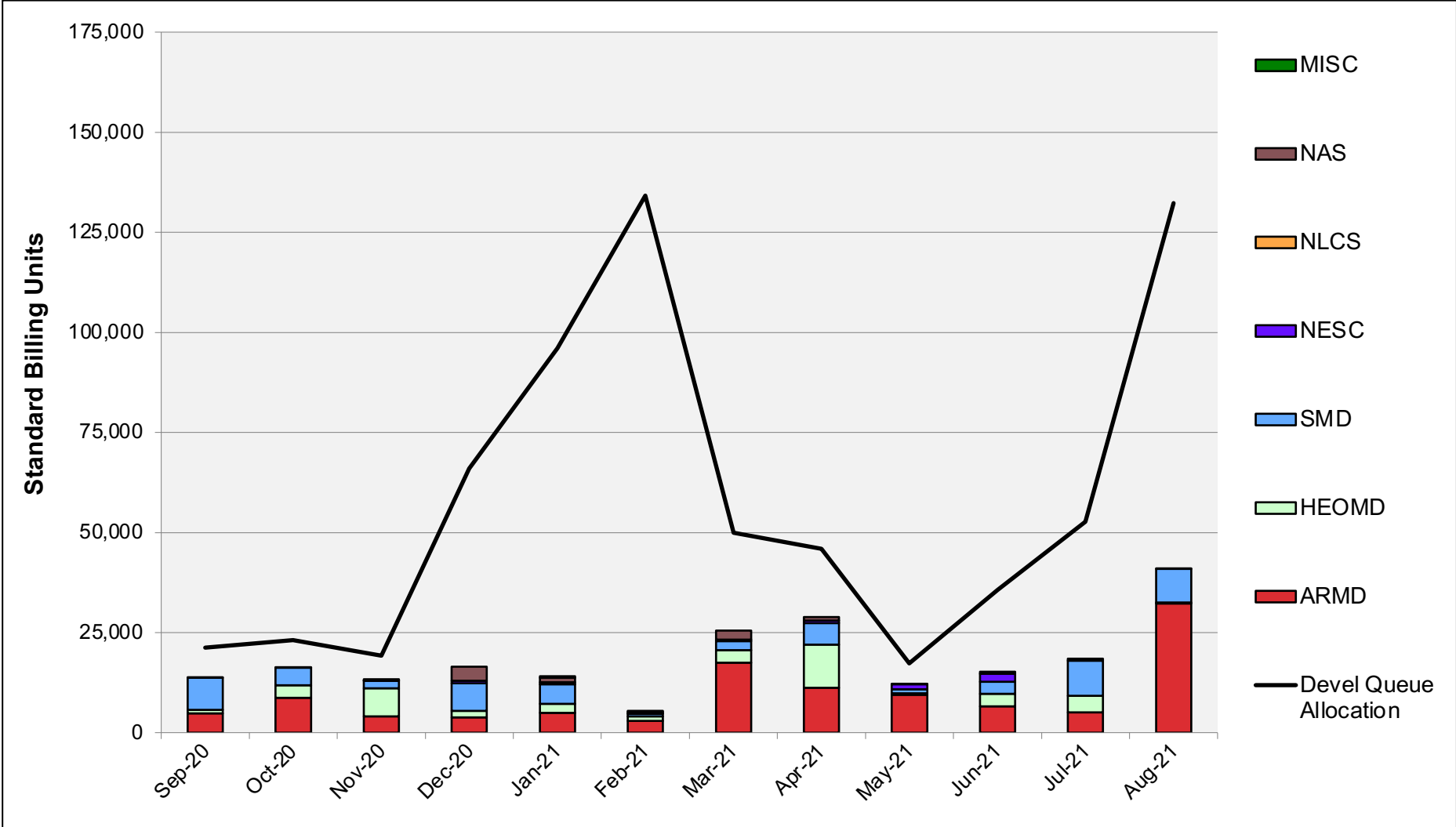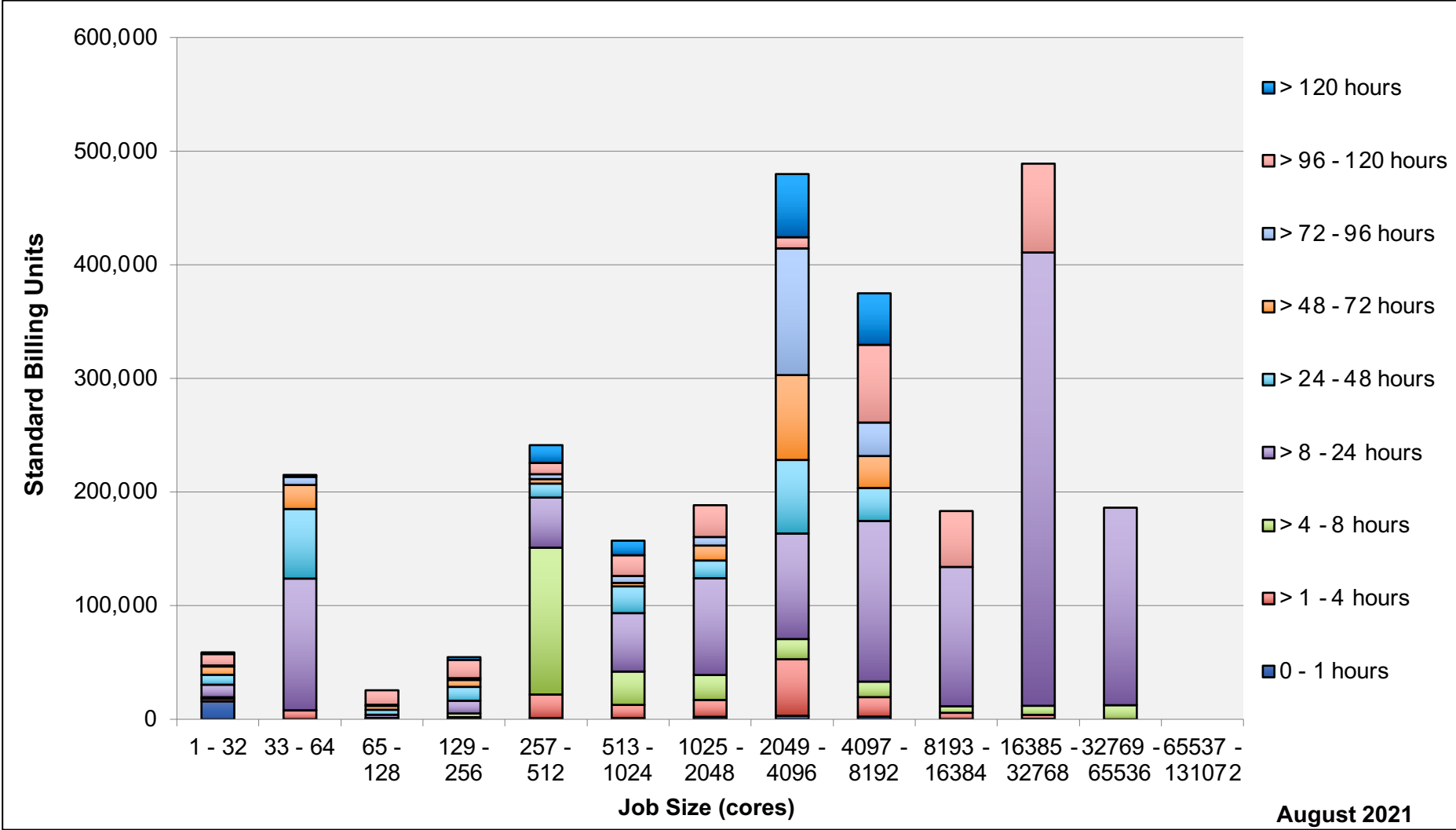
Aitken: Monthly Utilization by Job Length
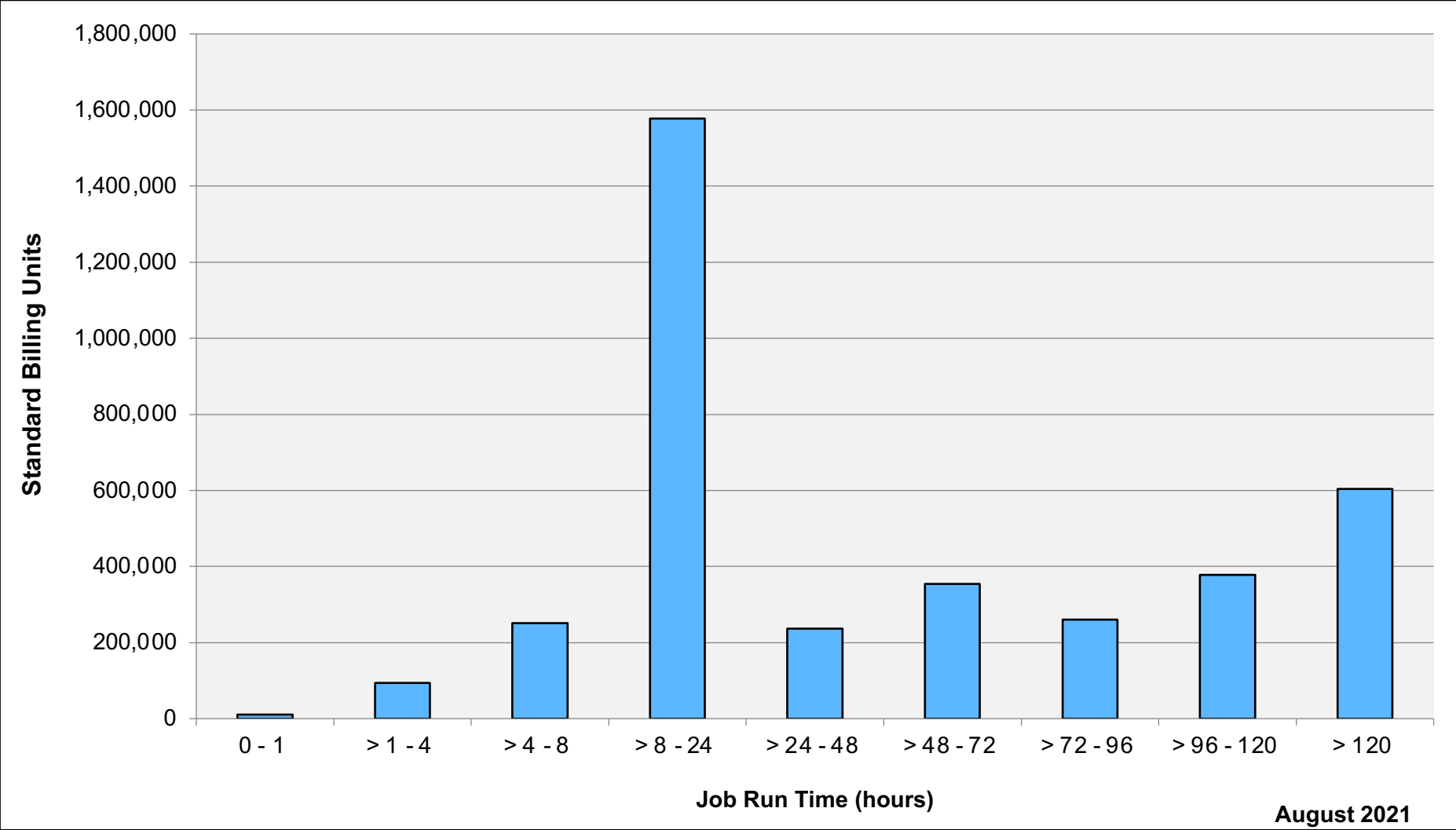
Chart showing Standard Billing Units versus Job Run Time (hours) for August 2021. Y-axis labeled "Standard Billing Units" ranging from 0 to 1,800,000. X-axis labeled "Job Run Time (hours)" with categories: 0 - 1, > 1 - 4, > 4 - 8, > 8 - 24, > 24 - 48, > 48 - 72, > 72 - 96, > 96 - 120, > 120.

August 2021

Aitken: Monthly Utilization by Job Size

August 2021

Aitken: Monthly Utilization by Size and Length

August 2021
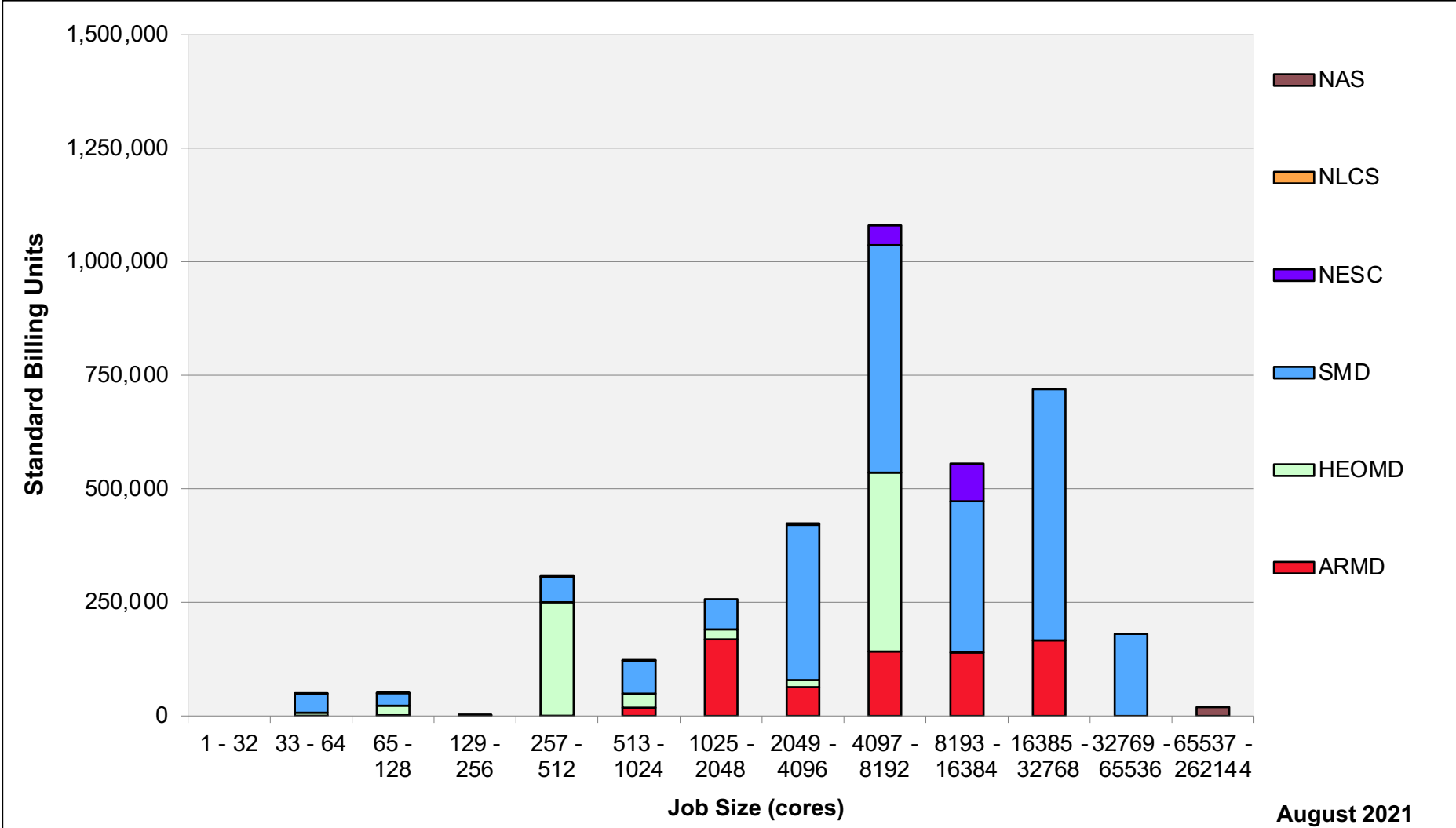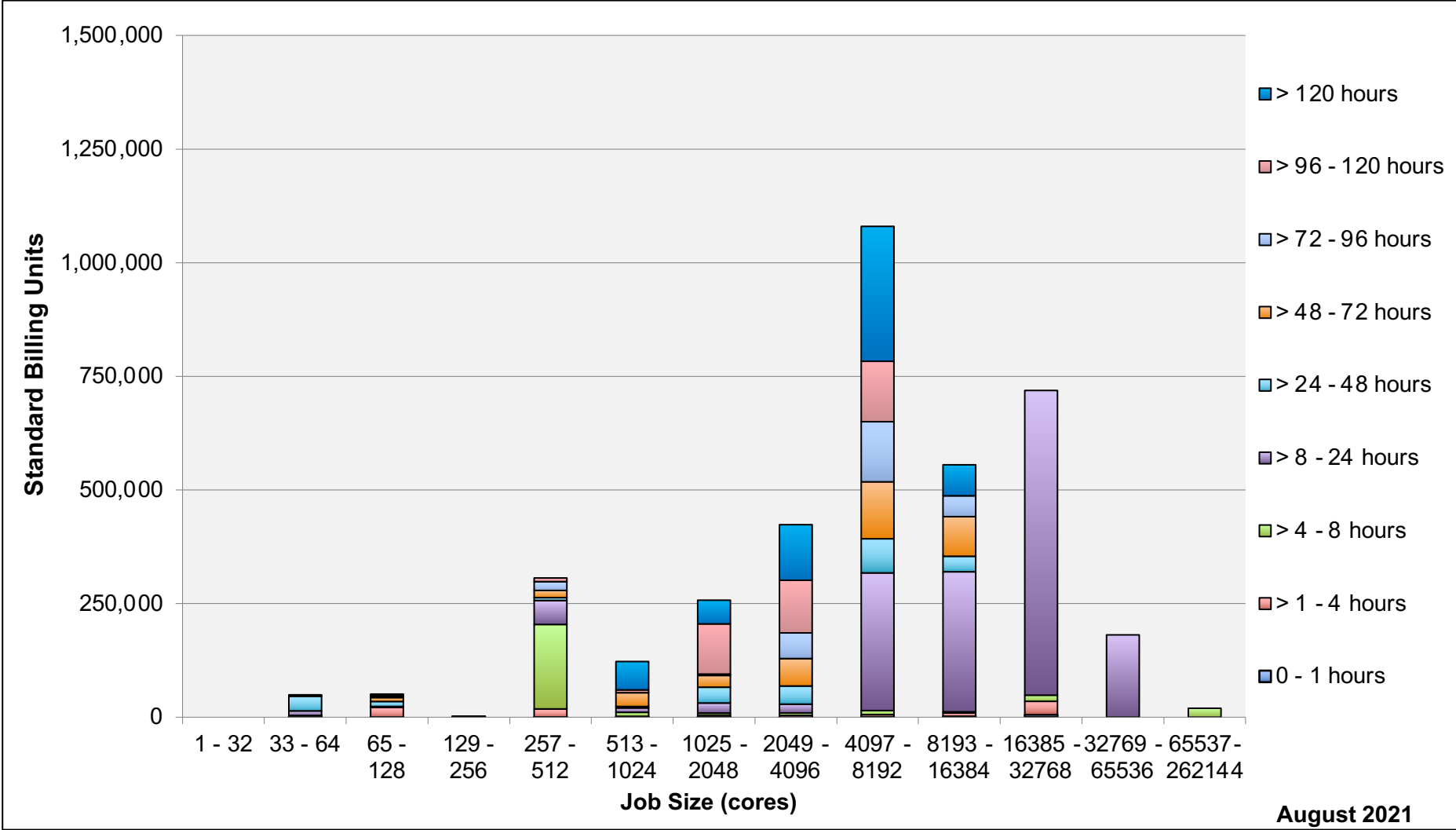
Aitken: Average Time to Clear All Jobs
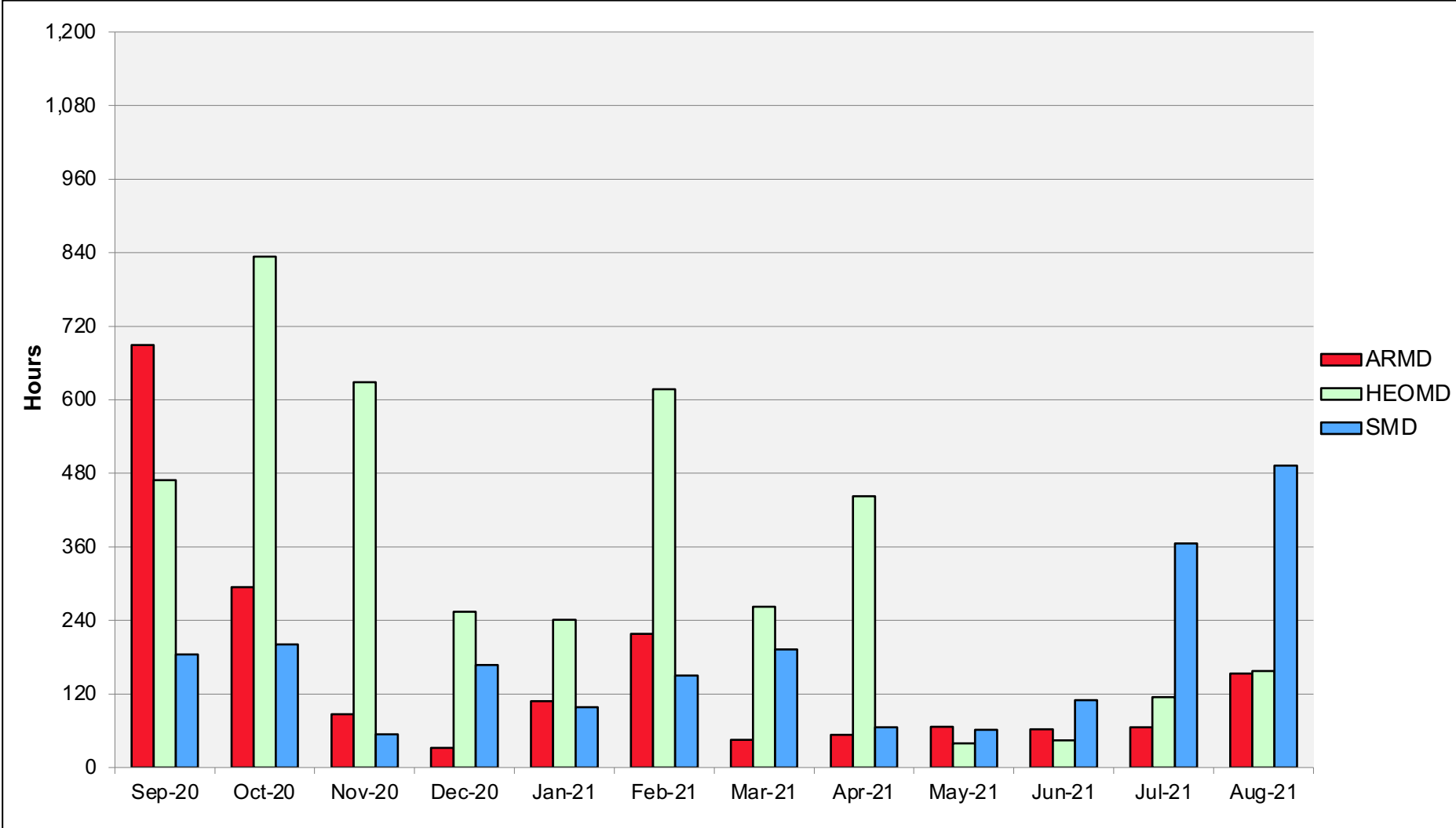
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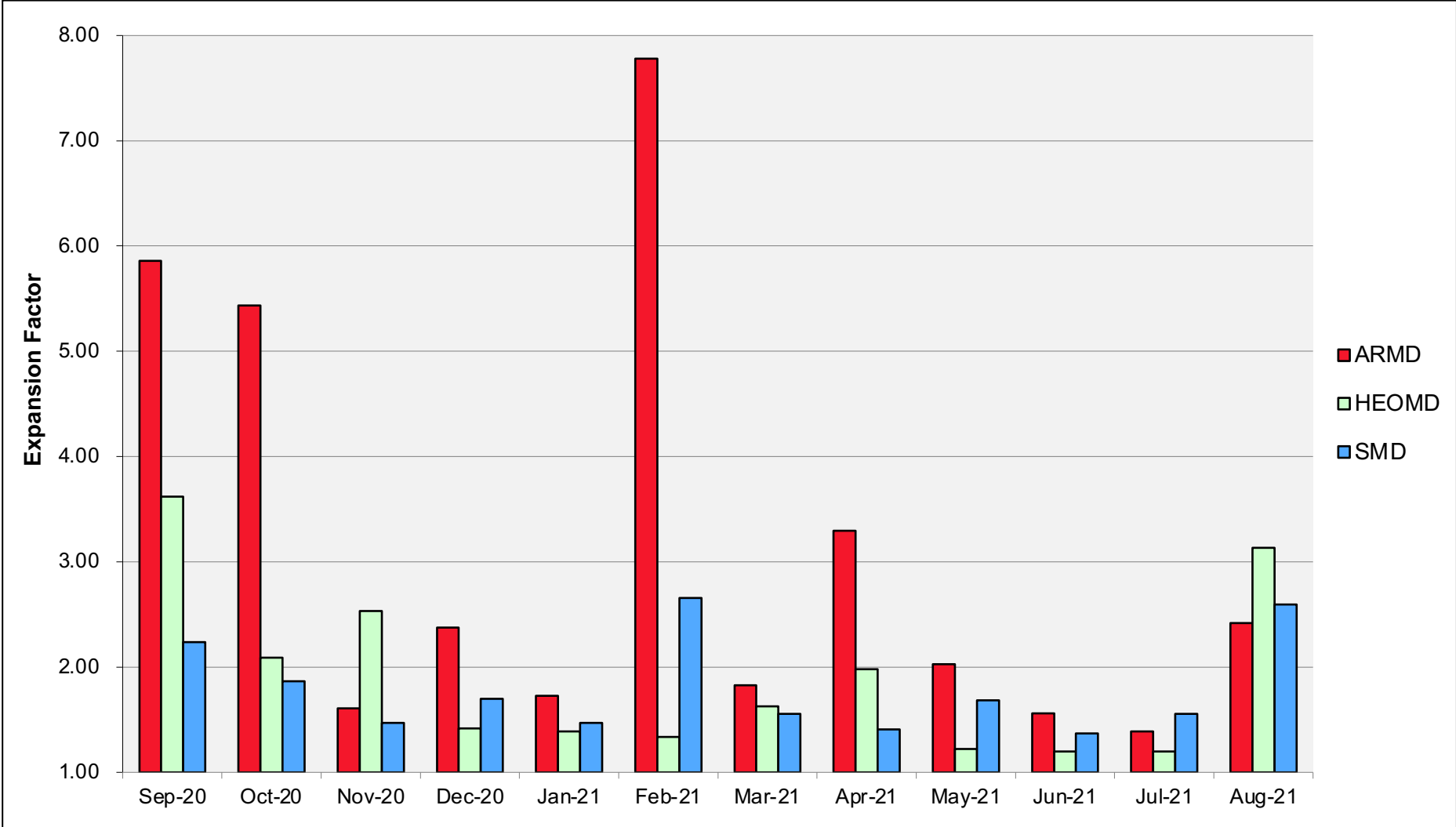
Electra: SBUs Reported, Normalized to 30-Day Month
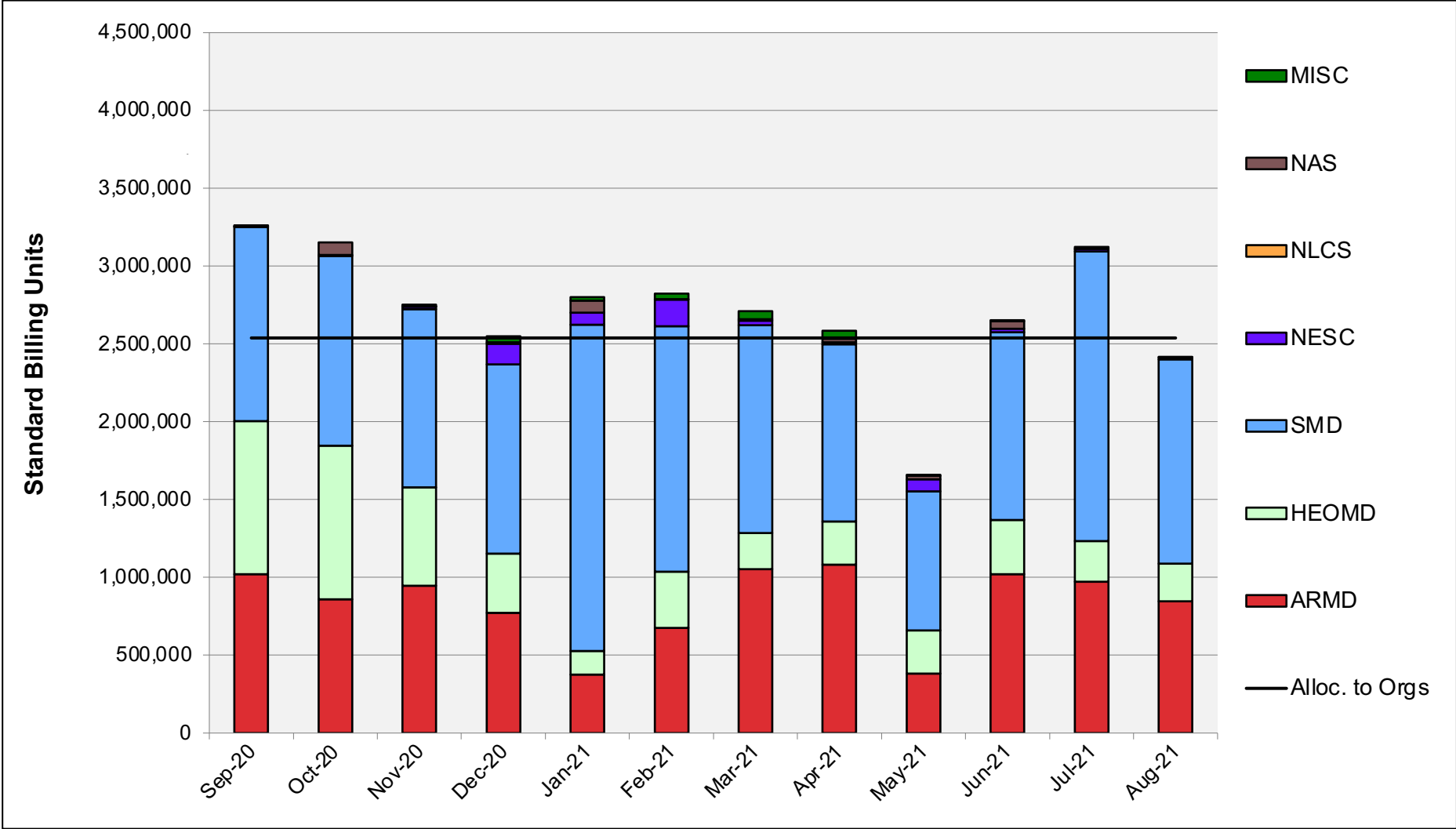
Electra: Devel Queue Utilization
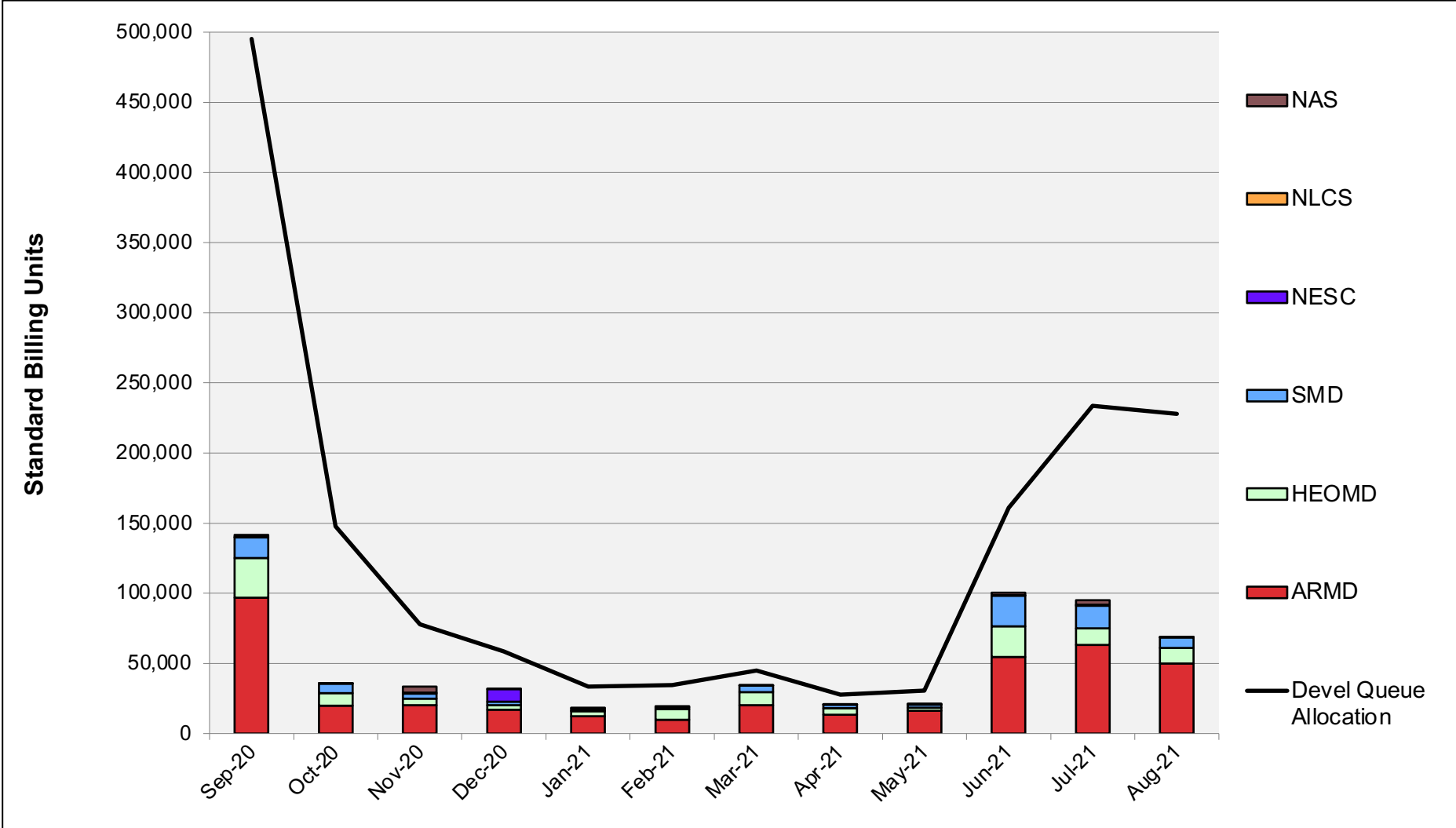
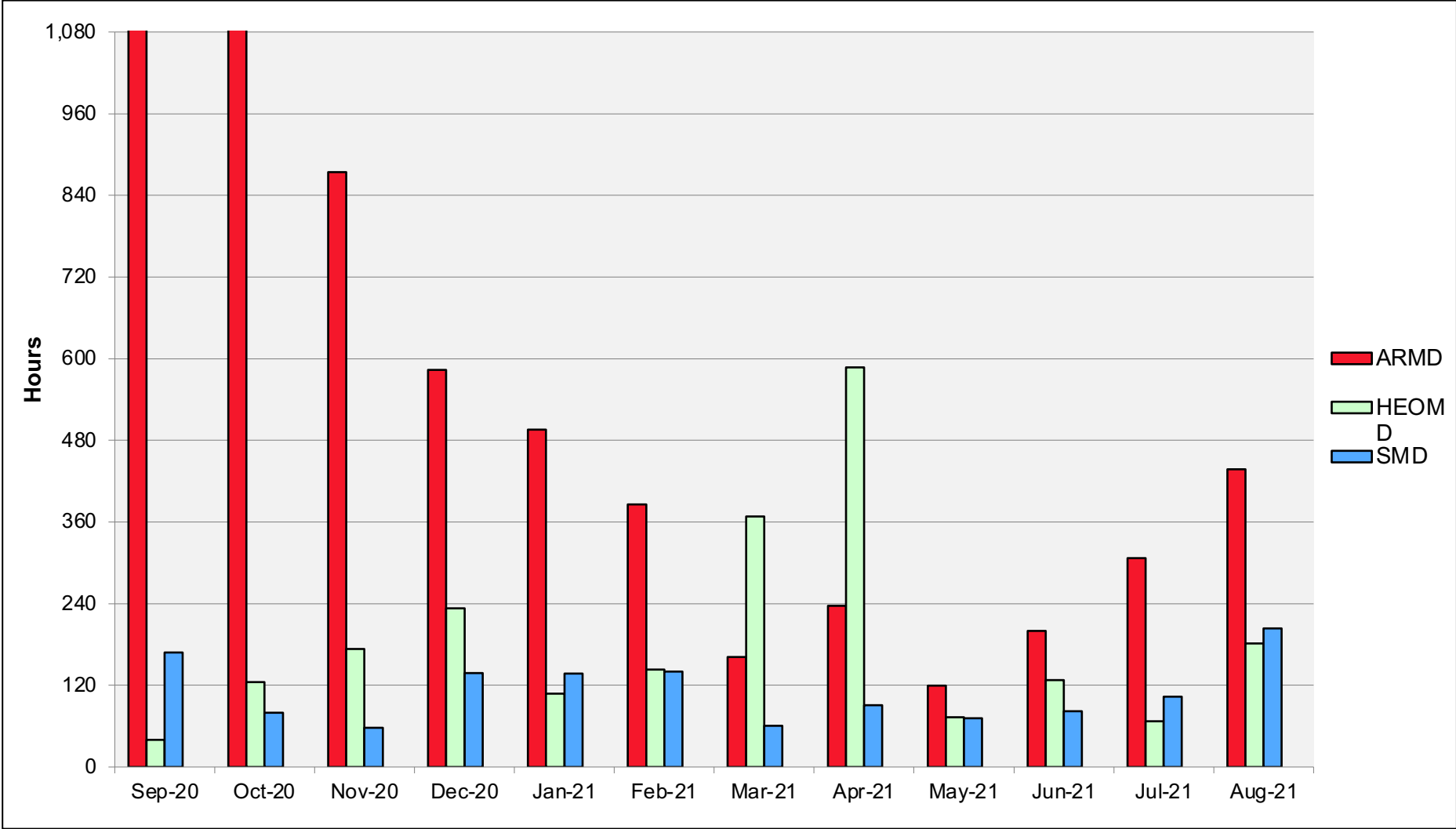# Electra: Monthly Utilization by Job Length
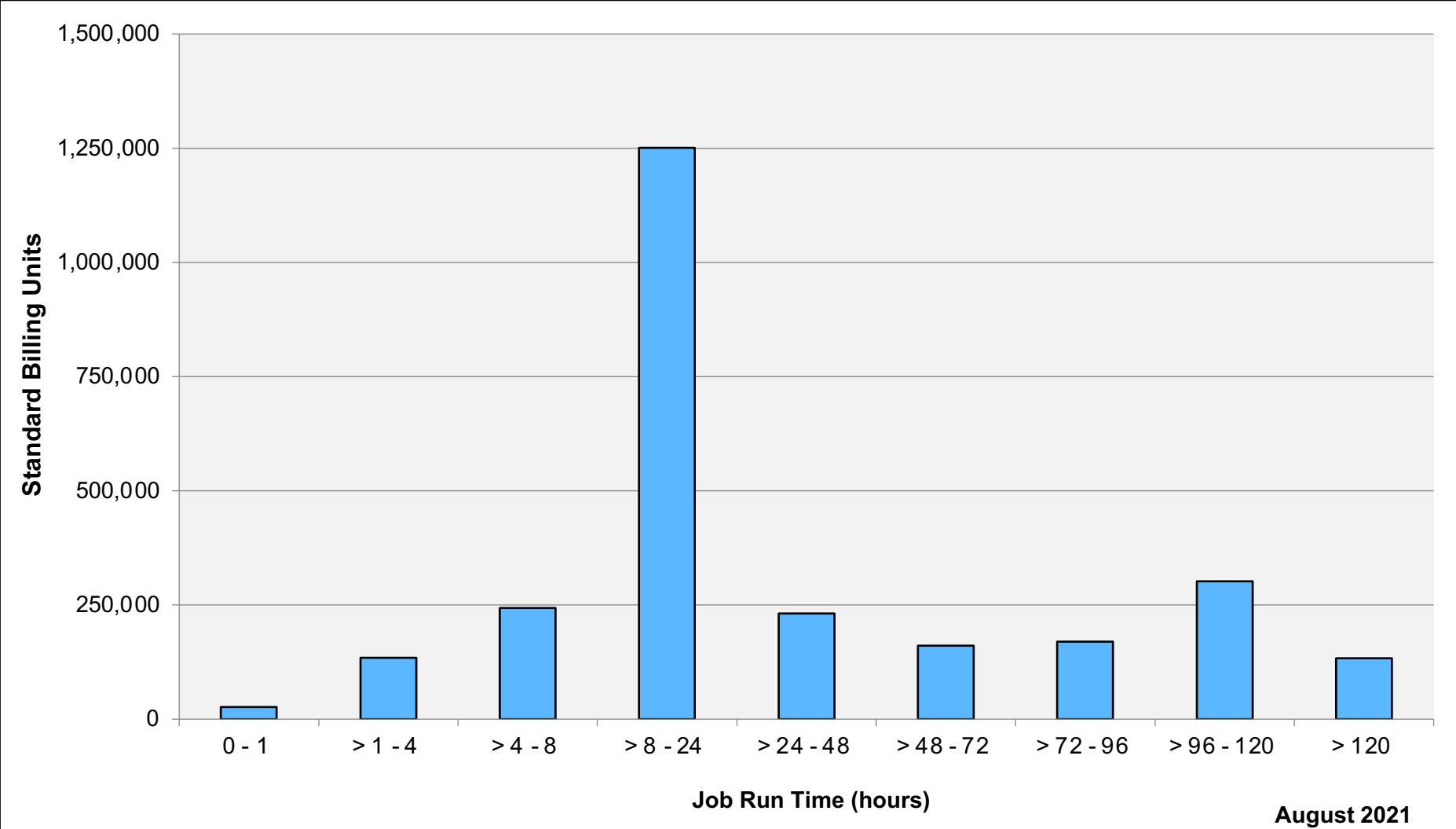
August 2021

Electra: Monthly Utilization by Job Size
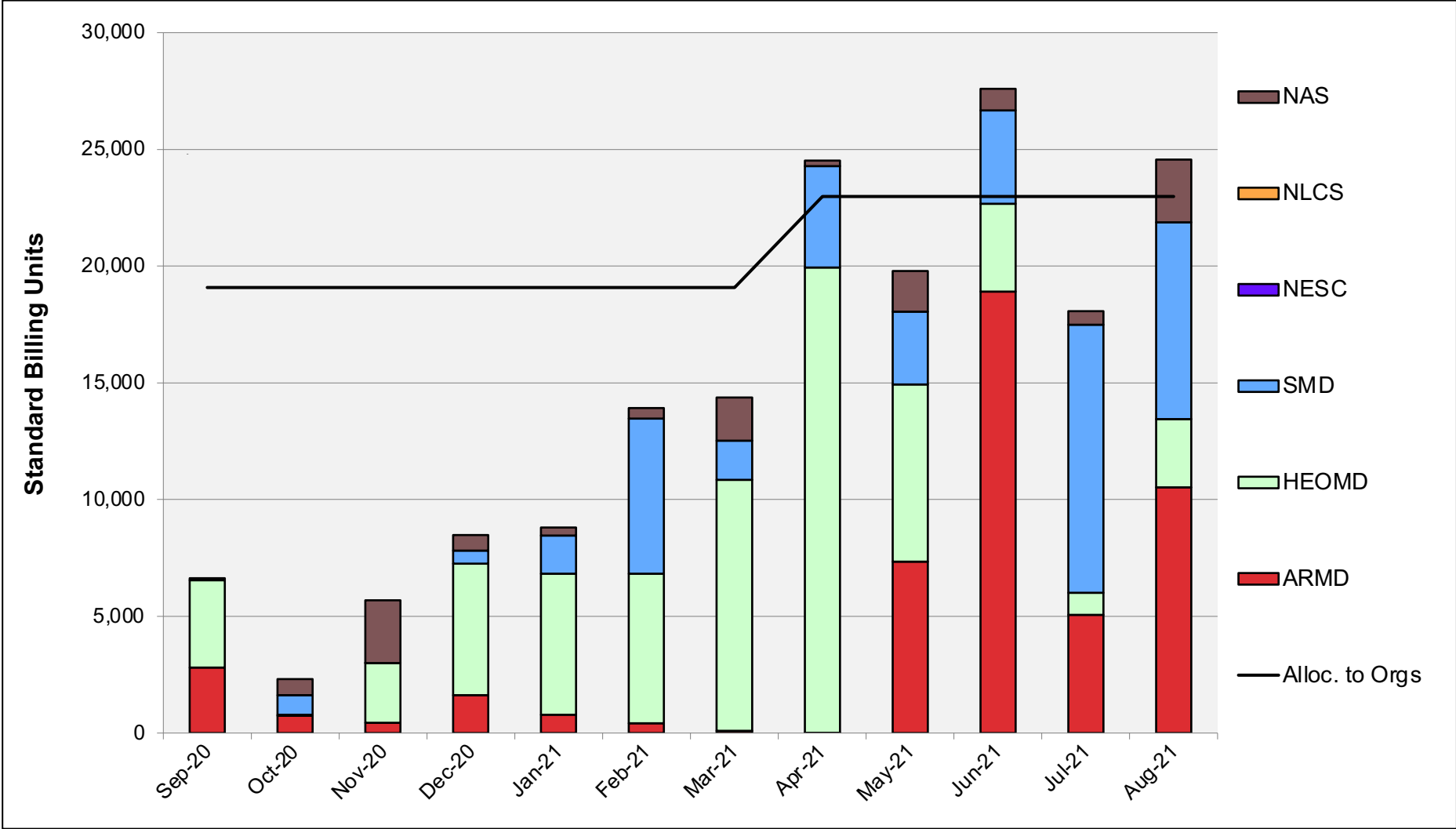

August 2021

Electra: Monthly Utilization by Size and Length

August 2021
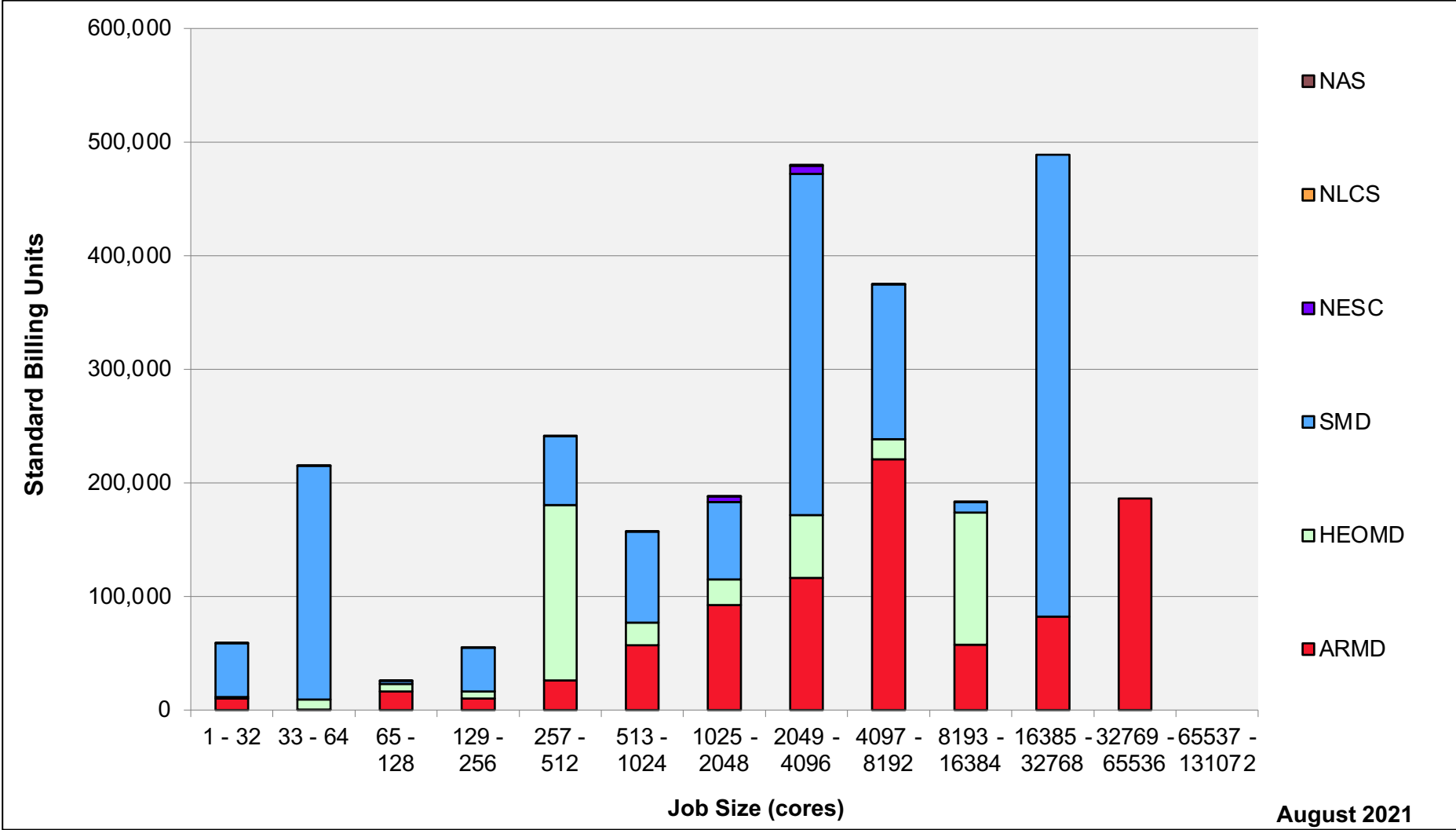
Electra: Average Time to Clear All Jobs
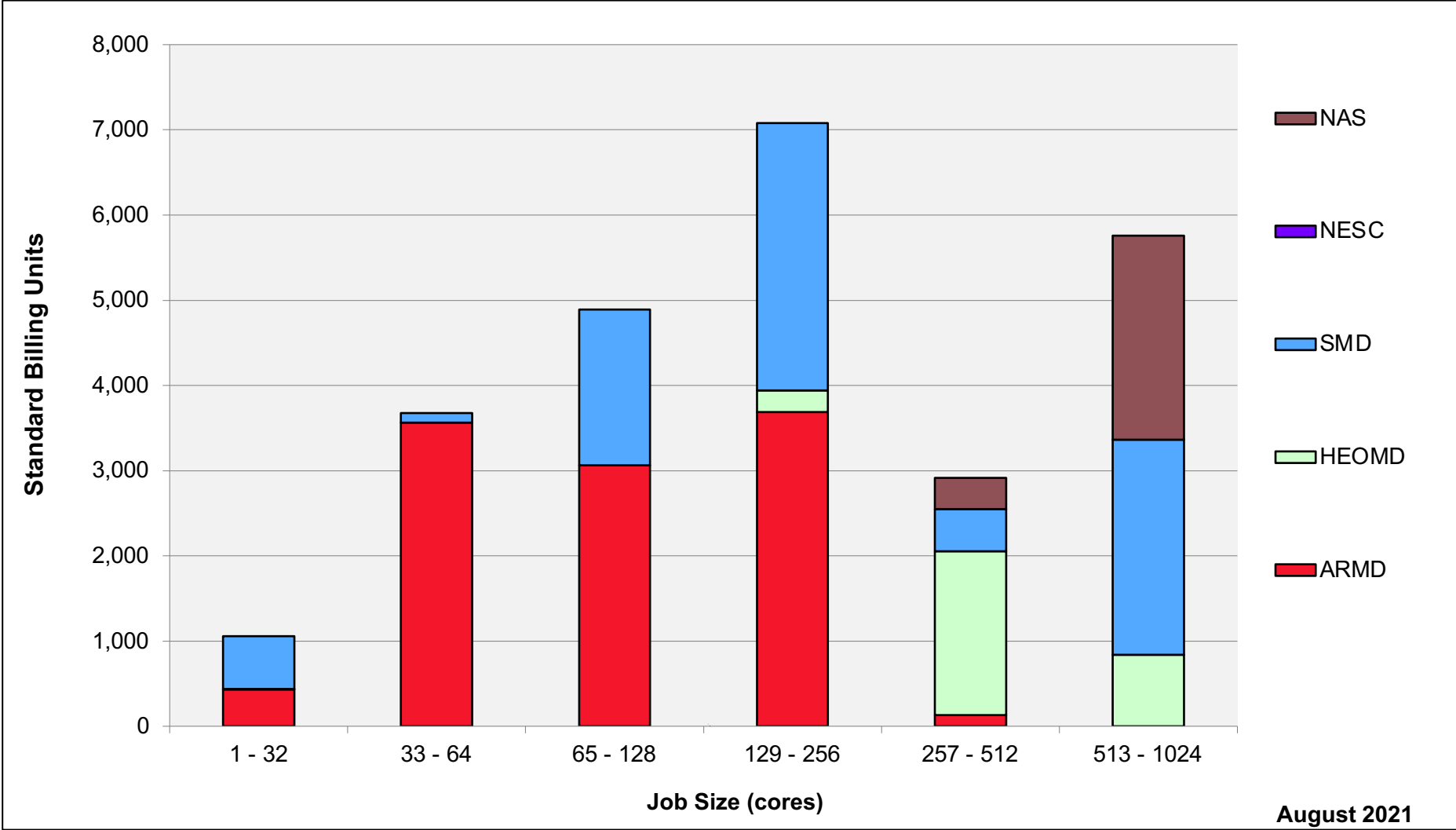
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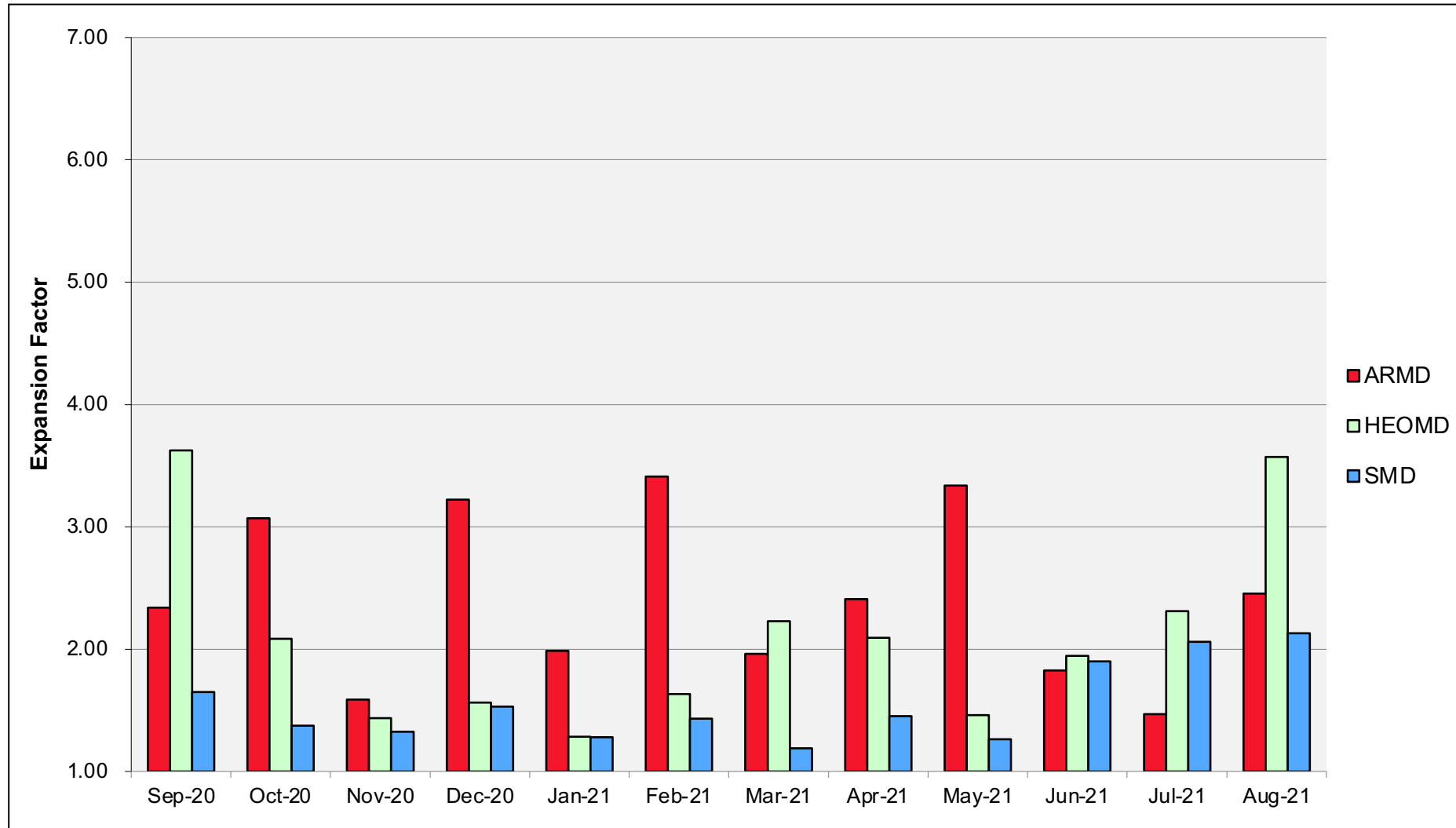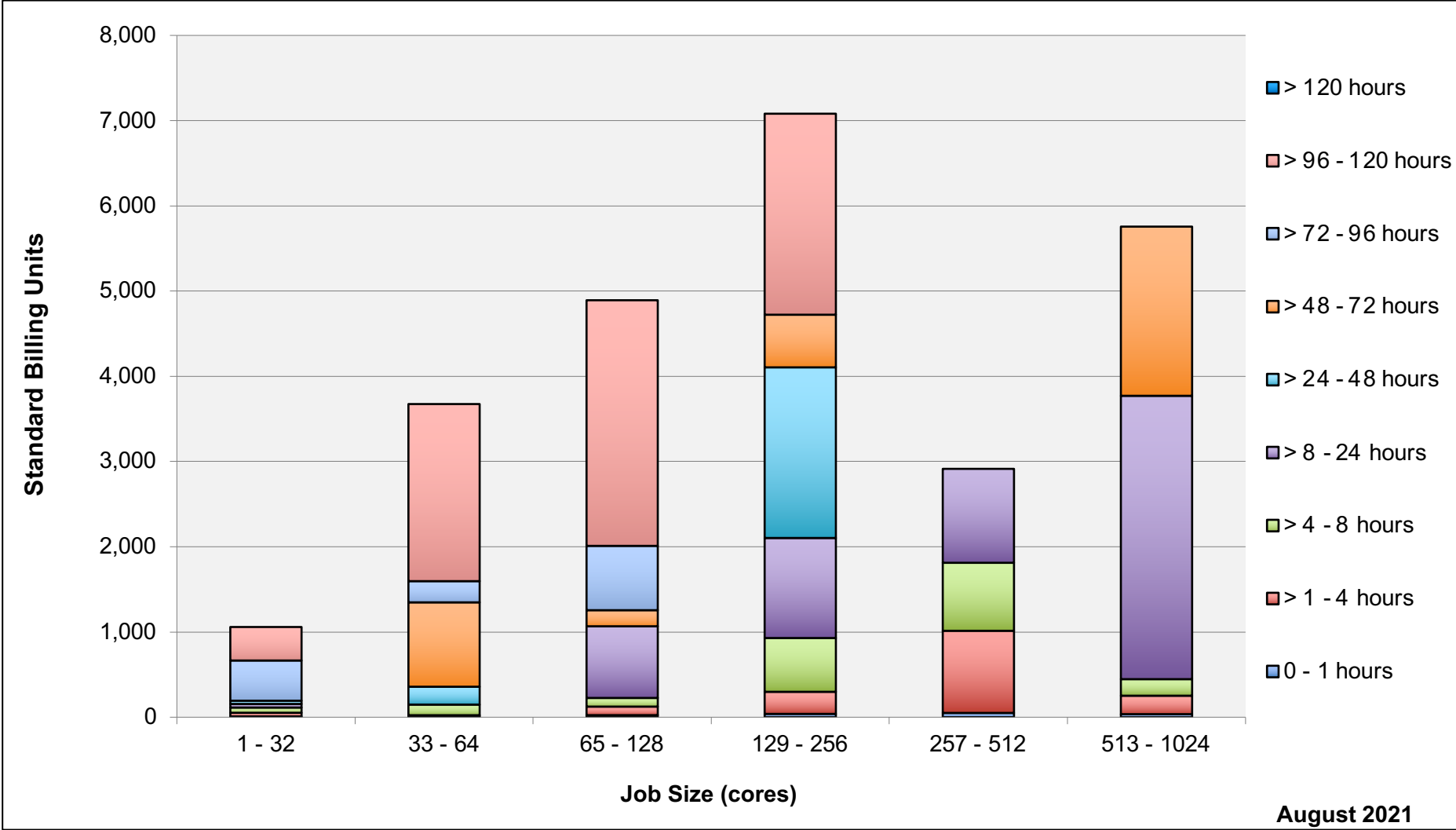
Endeavour: SBUs Reported, Normalized to 30-Day Month
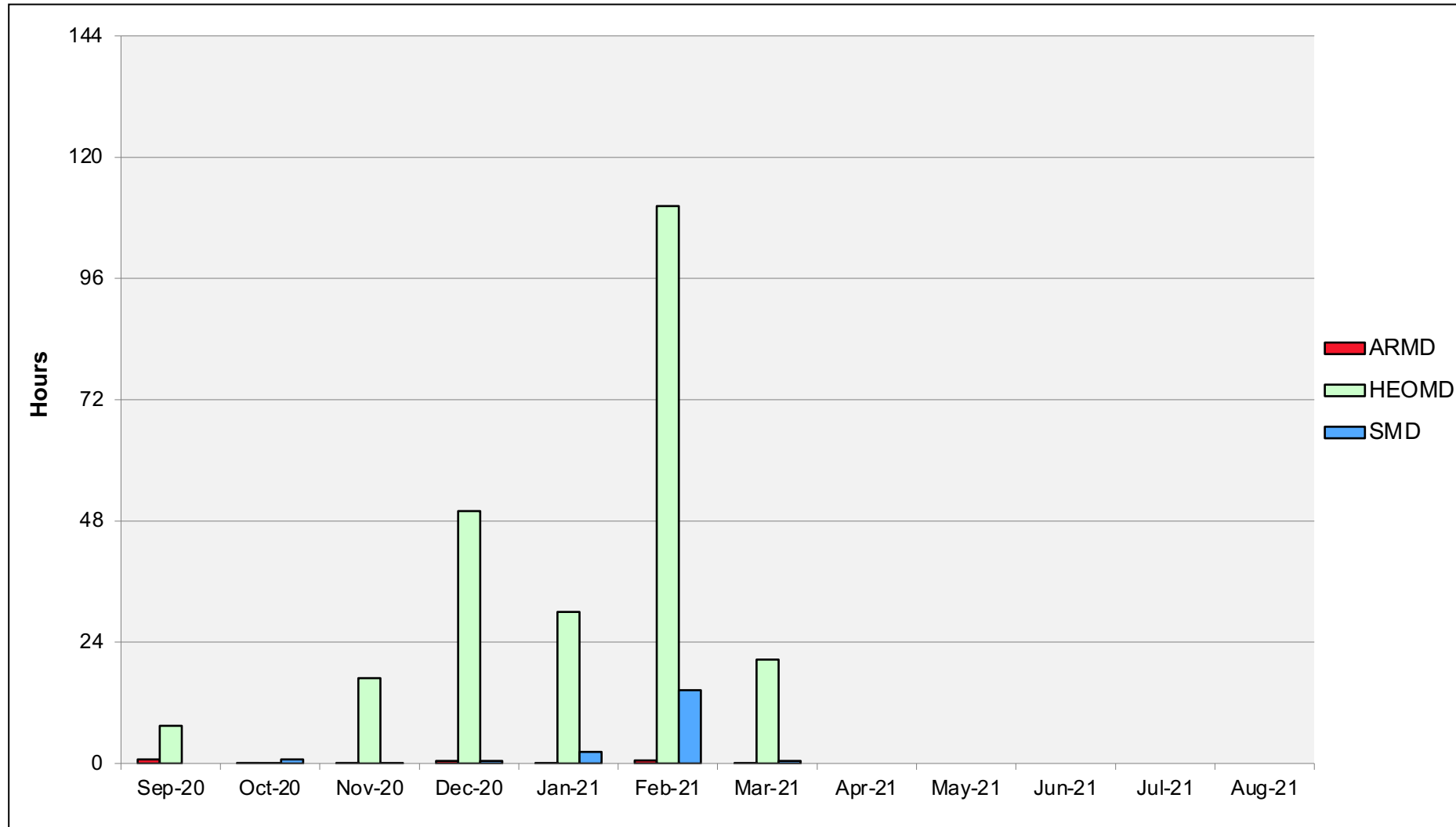
Endeavour: Monthly Utilization by Job Length
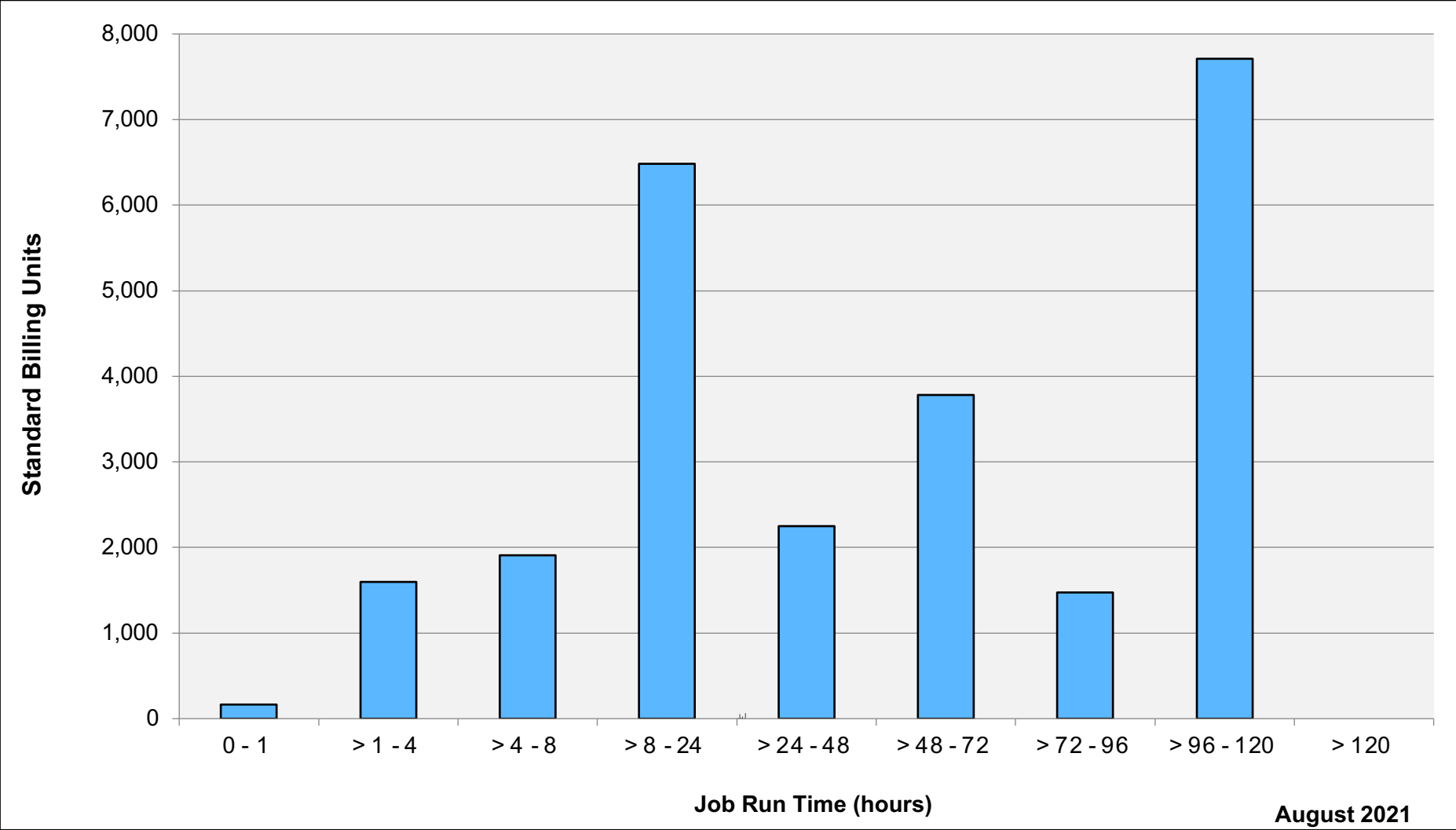
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August 2021

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Endeavour: Average Time to Clear All Jobs

September 10, 2021

Endeavour: Average Expansion Factor